# Finite-temperature density-functional theory of Bose-Einstein condensates

Nathan Argaman
*Physics Department, NRCN, P. O. Box 9001, Beer-Sheva 84190, Israel*

Y. B. Band
*Department of Chemistry, Department of Electro-Optics, and the Ilse Katz Center for Nano-Science, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel*

(Received 17 August 2010; published 18 February 2011)

The thermodynamic approach to density-functional theory (DFT) is used to derive a versatile theoretical framework for the treatment of finite-temperature (and in the limit, zero-temperature) Bose-Einstein condensates (BECs). The simplest application of this framework, using the overall density of bosons alone, would yield the DFT of Nunes [J. Phys. B **32**, 4293 (1999)]. It is argued that a significant improvement in accuracy may be obtained by using additional density fields: the condensate amplitude and the anomalous density. Thus, two advanced schemes are suggested, one corresponding to a generalized two-fluid model of condensate systems, and another scheme, which explicitly accounts for anomalous density contributions and anomalous effective potentials. The latter reduces to the Hartree-Fock-Bogoliubov approach in the limit of weak interactions. For stronger interactions, a local-density approximation is suggested, but its implementation requires accurate data for the thermodynamic properties of *uniform* interacting BEC systems, including fictitious perturbed states of such systems. Provided that such data become available (e.g., from quantum Monte Carlo computation), DFT can be used to obtain high-accuracy theoretical results for the equilibrium states of BECs of various geometries and external potentials.

DOI: 10.1103/PhysRevA.83.023612 PACS number(s): 03.75.Hh, 67.85.−d, 71.35.Lk

## I. INTRODUCTION

Our understanding of quantum-degenerate dilute Bose gas systems has increased dramatically since the experimental achievement of Bose-Einstein condensation (BEC) in ultracold dilute alkali gases in 1995 [1–3]. The explosive growth of knowledge of these systems has enriched both atomic-molecular-optical physics and many-body physics. Landmark developments include the realization of control over the interaction strength through magnetic-field tuning of a Feshbach resonance [4,5], the generalization for fermion systems, where the crossover between BCS-type and BEC superfluidity has been observed [6], nonlinear atom optics [7], mixed-phase condensates with different hyperfine states [8,9], mixtures of different bosonic atoms (e.g., Na-Rb) [10], mixed Bose-Fermi ultracold dilute-gas systems [11,12], and studies where optical potentials have been imposed on condensate systems, including systems in optical lattices, which are analogous to condensed-matter systems with either weak or strong correlations [13]. In the present paper, advanced methods for evaluating the finite-temperature equilibrium properties of a single-component dilute system of degenerate bosonic atoms in an external potential will be studied.

A dilute gas of atoms behaves classically as long as the thermal de Broglie wavelength $\lambda_T = \sqrt{2\pi\hbar^2/mk_BT}$ is smaller than the mean spacing between atoms $n^{-1/3}$, where $T$ is the temperature, $n$ is the gas density, and $m$ is the atomic mass. Quantum degeneracy for a gas of bosonic atoms ensues when the atomic wave packets begin to overlap (i.e., when $\lambda_T \gtrsim n^{-1/3}$), and a condensate becomes populated. For a uniform noninteracting bosonic system, the critical temperature $T_c$ is given by the condition $n\lambda_T^3 = \zeta(3/2) \simeq 2.612$, where $\zeta$ is the Riemann $\zeta$ function. As the temperature is lowered further, the kinetic energy of a uniform noninteracting gas decreases and vanishes in the $T \to 0$ limit. For a trapped noninteracting gas, all the bosons occupy the ground state in this limit, with the zero-point kinetic energy density balancing that of the external potential.

In realistic Bose-Einstein-condensed systems, interactions cannot be ignored, as the interaction-energy density is typically not small compared with the kinetic-energy density (or with that of the external potential). For systems that are dilute enough for the mean spacing between atoms to be much larger than the range of the atomic potential [14], the interactions can be well modeled with a contact interaction with an effective coupling constant $g = 4\pi\hbar^2 a_0/m$, which is proportional to the two-body $s$-wave scattering length $a_0$ (see Ref. [15]). At zero temperature, the strength of the interactions is quantified by the gas parameter $na_0^3$. In many practical applications, this parameter is very small because $a_0$ is of nanometer scale, whereas, the density of the alkali atoms at the moment of condensation is on the order of several atoms per cubic micrometer. A reasonably good description of such systems can be obtained by using the first-order expression for the interaction energy. Nevertheless, for high accuracy, terms beyond the first order should be taken into account because the density at the center of the trap increases dramatically as the system is cooled below the condensation temperature and because the relative magnitude of the leading correction is of order $10\sqrt{na_0^3}$ rather than of order $na_0^3$. Furthermore, the value of $a_0$ can be made much larger near a Feshbach resonance, driving the system into a strongly interacting regime. At finite temperatures, the effects of the interactions are more involved as the ratio $gn/k_BT$ is also an appropriate measure of the strength of the interactions in addition to the gas parameter. If the gas parameter is small, this ratio also is small at the transition temperature, but it can become arbitrarily large upon decreasing the temperature.

 

In this paper, a finite-temperature density-functional theory (DFT) approach to treat degenerate bosonic gases is developed. It is well known that DFT provides both a rigorous conceptual framework and a set of highly accurate practical tools for calculating the ground-state properties of interacting electron systems (for an introduction to DFT, see Refs. [16–18]). Today, most calculations of the electronic structure of atoms, molecules, and solids are carried out using the Hohenberg-Kohn-Sham DFT approach introduced in the 1960s [19,20]. DFT has been generalized in many ways, e.g., to treat systems at finite temperature [21], systems subject to time-dependent external fields [22–24], superconducting electronic systems [25], and systems as diverse as nuclei [26], classical fluids [27], spin-density waves [28], and superfluid liquid He [29,30]. Another development in DFT is the suggestion of using the principles of equilibrium thermodynamics to establish the finite-temperature version of DFT as a fundamental thermodynamic representation of the free energy, viewing the ground-state DFT as the $T \to 0$ limit of this representation [17,31]. Here, we follow this approach and apply it to dilute-gas bosonic systems.

DFT is a method for calculating the energy and density distribution of an inhomogeneous system. Within the Kohn-Sham approach, it employs a noninteracting reference system, which has the same density distribution $n(\mathbf{r})$ as the fully interacting system. This noninteracting system is associated with an effective potential, which is distinct from the external potential of the interacting system. The effects of the interactions may be included in a local approximation, which involves a simple integral over space and, at each point $\mathbf{r}$, accounts for the difference in energy per particle between *homogeneous* noninteracting and interacting systems of density $n(\mathbf{r})$ (for electrons, a Hartree term is used to account for the long-range part of the Coulomb interactions). Moreover, for electrons at zero temperature, this difference in energy between homogeneous systems can be described by the well-known Wigner interpolation formula [32] or the Gunnarsson-Lundqvist formula [33], and precise quantum Monte Carlo calculations are available [34]. Although the local-density approximation (LDA) already achieves surprisingly high accuracy for many electronic systems, an even higher precision is required for applications, e.g., in chemistry, motivating the ongoing development of more sophisticated approaches. Note that DFT is not, in principle, a method for calculating the excitation spectra of the systems studied, although the spectrum of the Kohn-Sham reference system often fits the spectrum of the interacting system quite well (DFT has even become a standard tool for evaluating band structure for electrons in periodic crystals, although, in principle, it is only a zeroth-order approximation in the context of the methods devised for calculating such quantities, such as the GW method [35]).

In response to the above-mentioned experimental developments, several authors developed DFT methods for dilute-gas bosonic systems. An early attempt to develop a DFT with a high-accuracy Bogoliubov-type treatment of the Kohn-Sham system was made in Ref. [36], which employs both the density distribution $n(\mathbf{r})$ and the condensate amplitude $\Phi(\mathbf{r})$ as functional variables. According to the analysis to be described here, such a high-level treatment actually requires the use of three independent functional variables, as discussed in Sec. VI. A straightforward application of DFT to boson systems, based on the density $n(\mathbf{r})$ alone, was suggested by Nunes [37]. For ground states (i.e., at $T = 0$), this approach results in a modified Gross-Pitaevskii (G-P) equation, containing terms that are nonlinear in the coupling constant $g$. It has been applied to experimentally relevant regimes [38] and generalized, e.g., for time-dependent potentials [39], and to address issues particular to strictly one-dimensional systems [40]. The possibility of a generalization for finite temperatures was noted by Nunes [37], but it is inferior compared to the two-fluid approach [41] (not to be confused with the Landau two-fluid approach to superfluids), which was already available at the time. Specifically, the two-fluid approach achieves improved accuracy by treating the condensate component $\Phi$ and the thermal component $n - |\Phi|^2$ separately, with the two components subject to different potentials (the interplay between the two components can also be studied experimentally [42]). Note, however, that Ref. [41] considered large systems with very weak inhomogeneities, for which finite-size effects are negligible, and one may assume local thermodynamic equilibrium. For such weakly inhomogeneous systems, application of a sophisticated DFT is superfluous. Also note that the two-fluid approach is less accurate than the field-theoretic approach in the Popov approximation, which was applied at roughly the same time [43].

Two different versions of DFT for bosons will be presented in what follows, based on the systematic thermodynamic approach. One version is based on treating the total density $n = \langle \hat{\psi}^\dagger \hat{\psi} \rangle$ and the condensate amplitude $\Phi = \langle \hat{\psi} \rangle$ as two density components. Correspondingly, the Kohn-Sham reference system is a noninteracting boson system, which has the same $n(\mathbf{r})$ and $\Phi(\mathbf{r})$ distributions and is subject not only to an effective noninteracting potential $v_{\rm ni}(\mathbf{r})$, but also to a fictitious potential $\eta_{\rm ni}(\mathbf{r})$, which couples directly to the condensate amplitude $\Phi(\mathbf{r})$. This version, which may be called $\Phi$-DFT, reduces to the two-fluid approach of Ref. [41] in the limit of weak interactions and large systems. It allows for inclusion of appropriate nonlinear-in-$g$ terms for stronger interactions as well as application to systems with significant inhomogeneities. The second version treats the anomalous density $\Delta = \langle \hat{\psi} \hat{\psi} \rangle$ as a third density, resulting in a Kohn-Sham system, which is also subject to an anomalous potential $\xi_{\rm ni}(\mathbf{r})$, for which a generalized Bogoliubov-type treatment is appropriate. This version is referred to as anomalous DFT (A-DFT) and bears some resemblance to the electronic DFT devised for superconducting systems [25]. In the limit of weak interactions, it reproduces the Hartree-Fock-Bogoliubov model (a further approximation to which yields the Popov model [44]).

In order to apply an LDA for the interaction effects, one needs results for uniform systems, as discussed previously. For dilute Bose gases, some results as a function of the density $n$ are available at both vanishing [37,45] and finite [44,46–48] temperatures. However, application of the advanced DFT versions discussed in the following requires generalization of these results to functions not only of the density, but also of the condensate amplitude for $\Phi$-DFT and of the anomalous density for A-DFT. These generalized interacting systems are analogous to spin-polarized uniform electronic systems, data for which is in standard use within the LDA for electrons.

The difference is that manipulating the condensate amplitude $\Phi$ or the anomalous density $\Delta$ requires the use of fictitious potentials, whereas, the spin density can be modified by subjecting the system to a physically realizable magnetic field. As the uniform systems that are under consideration are fictitious anyway, and the results are obtained by theoretical methods (such as the quantum Monte Carlo work mentioned earlier [34]), the realizability or not of the fields is of little importance. Obtaining high-accuracy results for the generalized uniform systems is beyond the scope of the present paper, and, at this stage, we will content ourselves with expressions for the interaction effects, which are valid for first order in $g$ (for A-DFT, this corresponds to the Hartree-Fock-Bogoliubov model as noted previously), with one exception: The leading-order results for A-DFT will allow us to deduce next-to-leading-order results for $\Phi$-DFT (see Sec. V). For dilute gases, the first-order approximation to A-DFT is wholly sufficient, except for special cases with particularly strong interactions, which are realizable near Feshbach resonances [4,5]. It is also relevant to note that homogeneous systems with attractive interactions (negative scattering lengths $a_0$) are absolutely unstable at long wavelengths, but inhomogeneous attractive systems may have metastable dilute-gas states and have been studied experimentally (see the last item in Ref. [5]). $\Phi$-DFT and A-DFT may be applied to such systems with the leading-order expressions for the interactions, whereas, a higher-accuracy local-density approach is, in principle, unworkable because there can be no accurate thermodynamic results for the relevant interacting homogeneous system (except at uninterestingly low densities, where thermal excitations stabilize the long-wavelength perturbations). The high-accuracy methods developed here are therefore limited primarily to systems with repulsive interactions.

The outline of the paper is as follows. Section II introduces the general formalism of DFT in the thermodynamic language. Section III presents $\Phi$-DFT: It applies the principles of DFT to nonuniform BECs, using the total density $n(\mathbf{r})$ and the condensate amplitude $\Phi(\mathbf{r})$ as free variables. The presentation includes the Thomas-Fermi approximation for the Kohn-Sham system, which is applicable when the inhomogeneities are weak, and the first-order approximation to the interaction energy. In Sec. IV, a more general DFT scheme is developed wherein, apart from $n(\mathbf{r})$ and $\Phi(\mathbf{r})$, the anomalous density $\Delta(\mathbf{r})$ also is used as a third free variable. In this case, the $O(g)$ approximation leads to the Hartree-Fock-Bogoliubov system. Here too, the Thomas-Fermi approximation is introduced. Section V demonstrates one of the advantages of A-DFT by showing how a result for a homogeneous system, which is available with its $O(g)$ approximation, can be obtained within $\Phi$-DFT only if more complicated higher orders are included. Section VI presents a discussion of this comparison, concluding remarks, and suggestions for future research.

## II. FINITE-TEMPERATURE DFT

The purpose of this section is to introduce the relevant concepts of DFT. The thermodynamic approach of Ref. [17] is followed and generalized to cases with several density distributions. This will allow not only the total density of particles $n(\mathbf{r})$, but also the condensate amplitude $\Phi(\mathbf{r})$ and the anomalous density $\Delta(\mathbf{r})$ to be used as free variables, as discussed before.

The Hamiltonian of the inhomogeneous system may be written as $\hat{H} = \hat{H}_{\rm ni} + \Lambda \hat{H}_{\rm int}$, where $\hat{H}_{\rm int}$ includes all the interaction terms and $\hat{H}_{\rm ni}$ is a noninteracting (quadratic in field-operators) Hamiltonian, for which accurate solutions are obtainable at an acceptable computational cost. $\Lambda$ is a continuous parameter specifying the strength of the interactions, with $\Lambda = 1$ for the full interacting system and $\Lambda = 0$ for the noninteracting case. The single-particle fields specifying the inhomogeneity, such as the potential terms containing the external potential $v(\mathbf{r})$ and other fields $\mathbf{B}(\mathbf{r})$, are included in $\hat{H}_{\rm ni}$, and these couple to the densities $n(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$, respectively. In the interest of generality, the exact nature of $\mathbf{B}(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$ will not be specified yet, but as an example, one may keep in mind electrons in a magnetic field $\mathbf{B}(\mathbf{r})$, which couples to the spin density (magnetization) $\mathbf{m}(\mathbf{r})$ [31].

The focus of this section is the thermodynamic treatment. The statistical-physics problem of obtaining the grand potential $\Omega$ from the Hamiltonian $\hat{H}$ will be tackled in Secs. III and IV, where specifics of the Hamiltonian for bosons will be given. In Sec. II A, the foundation of DFT will be laid out, by explaining how the densities (rather then the external fields) can be regarded as the free functional variables, which specify the inhomogeneous system. This is a direct generalization of Legendre transforms [i.e., of the replacement of one free variable (e.g., the chemical potential $\mu$) by another (e.g., the total number of particles $N$)]. Section II B explains how, within the DFT framework, the interacting system can be related to a specific Kohn-Sham noninteracting reference system and how the effects of interactions can be approximated, based on knowledge of homogeneous interacting systems (the LDA).

### A. Legendre transforms and the Hohenberg-Kohn theorems

Our starting point uses the grand potential $\Omega([v(\mathbf{r}) - \mu, \mathbf{B}(\mathbf{r})], T, \Lambda)$, which depends on the temperature $T$ and the chemical potential $\mu$ as well as the specifics of the Hamiltonian $\hat{H}$. The square brackets emphasize the functional character of $\Omega$ (i.e., the fact that its value depends on the potential, which is itself a function of position). The notation also makes explicit the fact that the grand potential depends only on the difference $v(\mathbf{r}) - \mu$, not the values of $v(\mathbf{r})$ and $\mu$ separately. The derivatives of the grand potential, with respect to its functional variables, are

$$n(\mathbf{r}) = \frac{\delta\Omega}{\delta v(\mathbf{r})}, \quad \mathbf{m}(\mathbf{r}) = -\frac{\delta\Omega}{\delta \mathbf{B}(\mathbf{r})}. \tag{1}$$

At this point, these equalities merely introduce notation for the derivatives; the fact that $n(\mathbf{r})$ really is the density will become evident in the statistical-physics discussion of Sec. III. The different signs used here are a matter of convention related to the fact that the potential $v(\mathbf{r})$ repels the density $n(\mathbf{r})$, whereas, the "magnetic field" $\mathbf{B}(\mathbf{r})$ attracts the "magnetic-moment" density $\mathbf{m}(\mathbf{r})$, as the magnetic energy density is given by $-\mathbf{m}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r})$.

We will use the fact that the grand potential $\Omega$ is concave in its functional variables, i.e., when it is evaluated at any two points $[v_1, \mathbf{B}_1]$ and $[v_2, \mathbf{B}_2]$ (at fixed $T > 0$, $\Lambda$ and $\mu$), and at their midpoint $[v_{1/2}, \mathbf{B}_{1/2}]$ with $v_{1/2} = \frac{1}{2}(v_1 + v_2)$,

$\mathbf{B}_{1/2} = \frac{1}{2}(\mathbf{B}_1 + \mathbf{B}_2)$, the mean of the values obtained at the two arbitrary points is strictly smaller than the value at the midpoint $\frac{1}{2}(\Omega_1 + \Omega_2) < \Omega_{1/2}$ (each one of these points is, of course, a set of functions of position, as appropriate for a functional). This property, along with others, which we will tacitly assume (e.g., differentiability of $\Omega$ for finite systems at finite temperatures) can be proven by statistical mechanics methods (incidentally, $\Omega$ is also concave in $\Lambda$ and $T$, but this will not be used here). The concavity of $\Omega$ guarantees that there exists a one-to-one relationship between the potentials and the densities. This corresponds to the first Hohenberg-Kohn theorem [19,21]. Thus, a particular inhomogeneous system can be identified by its densities $n(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$, instead of specifying the fields $v(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$.

It is convenient to demonstrate this graphically, together with the Legendre transforms to be introduced next, using one of the scalar variables of $\Omega$, the chemical potential $\mu$. The corresponding partial derivative of $\Omega$ is

$$N = -\frac{\partial \Omega}{\partial \mu}, \tag{2}$$

where $N = \int d\mathbf{r}\, n(\mathbf{r})$ is the total particle number. The one-to-one character of the relationship between $\mu$ and $N$ follows from the monotonic dependence of the derivative of $N$ with respect to the variable $\mu$, see Fig. 1. Next, consider the combination $\Omega(\mu) + \mu N$ and maximize it over all values of $\mu$ for a given $N$. The maximum is clearly unique because the combination is concave in $\mu$. By considering the derivative, one finds that, at the maximum, $\mu$ obeys the condition of Eq. (2). This maximum value of the combination is called the Helmholtz free energy,

$$F(N) = \max_{\mu} \Omega(\mu) + \mu N = \Omega(\mu) + \mu N|_{\mu:\, N(\mu)=N}. \tag{3}$$

The last equality refers to the equivalent procedure of choosing $\mu$ according to the condition of Eq. (2), rather than maximizing. The Legendre transform from $\Omega(\mu)$ to $F(N)$ has a simple geometric interpretation (see Fig. 1): The graph of $\Omega$ as a function of $\mu$ has tangents of slope $-N$, and, for a point $\Omega(\mu)$ on the graph, the intercept of the tangent line with the vertical axis occurs at $F(N) = \Omega + \mu N$.

The function $F(N)$, describing the family of tangents (intercept as a function of slope) for the curve $\Omega(\mu)$, contains the same information regarding the physical system as the original function $\Omega(\mu)$ but is, in certain applications, more

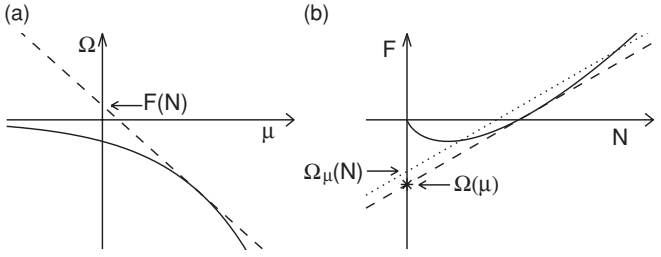


FIG. 1. (a) Legendre transform to obtain $F(N)$ from $\Omega(\mu)$ (see text). (b) Legendre transform back from $F(N)$ to $\Omega(\mu)$. The minimization procedure for the inverse Legendre transform is demonstrated in the second panel.

convenient. It follows, from Eq. (2), that the derivatives of $F$ are

$$\frac{\partial F}{\partial N} = \mu, \quad \left(\frac{\partial F}{\partial \Lambda}\right)_N = \left(\frac{\partial \Omega}{\partial \Lambda}\right)_\mu, \tag{4}$$

where the last equality represents a derivative with respect to a variable not involved in the Legendre transform. As $\mu$ increases with $N$, the function $F(N)$ is convex (it is concave relative to the other variables, $\Lambda$ and $T$). Thus, an inverse Legendre transform may be applied [e.g., by defining $\Omega_\mu(N) = F(N) - \mu N$ and by identifying the grand potential as $\Omega(\mu) = \min_N \Omega_\mu(N)$ (see the right panel in the figure)]. The inverse transform differs from the original Legendre transform only in signs.

In the case of functional variables, a geometric interpretation requires a multitude of horizontal axes (one for each spatial point) with high-dimensional tangent hyperplanes instead of tangent lines, but the principle is the same. Thus, the Hohenberg-Kohn free energy of DFT is introduced through a *functional* Legendre transform:

$$F_{\mathrm{HK}}([n,\mathbf{m}],T,\Lambda) = \Omega([v-\mu,\mathbf{B}],T,\Lambda) - \int d\mathbf{r}\,[(v-\mu)n - \mathbf{B}\cdot\mathbf{m}]. \tag{5}$$

Here, the functional variables $[v-\mu,\mathbf{B}]$ on the right-hand side (RHS) are determined by maximization or, equivalently, by requiring the physical condition of Eq. (1) (the argument $\mathbf{r}$ of the functions is omitted for brevity). The functional derivatives of $F_{\mathrm{HK}}$ are

$$\mu - v(\mathbf{r}) = \frac{\delta F_{\mathrm{HK}}}{\delta n(\mathbf{r})}, \quad \mathbf{B}(\mathbf{r}) = \frac{\delta F_{\mathrm{HK}}}{\delta \mathbf{m}(\mathbf{r})}. \tag{6}$$

The Hohenberg-Kohn free energy $F_{\mathrm{HK}}([n,\mathbf{m}],T,\Lambda)$ is the generalization of the Helmholtz free energy to inhomogeneous systems.

The inverse Legendre transform allows one to obtain the grand potential from the Hohenberg-Kohn free energy:

$$\Omega([v-\mu,\mathbf{B}],T,\Lambda) = F_{\mathrm{HK}}([n,\mathbf{m}],T,\Lambda) + \int d\mathbf{r}\,[(v-\mu)n - \mathbf{B}\cdot\mathbf{m}]. \tag{7}$$

Here, $n$ and $\mathbf{m}$ on the RHS are determined either by Eq. (6) or equivalently by minimization. The second Hohenberg-Kohn theorem corresponds to the latter statement: The RHS of Eq. (7), when evaluated for an interacting system ($\Lambda = 1$) at given external potentials $v = v_{\mathrm{ext}}(\mathbf{r})$ and $\mathbf{B} = \mathbf{B}_{\mathrm{ext}}(\mathbf{r})$ and minimized over the density distributions $n(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$, gives the physical value of the grand potential $\Omega$ at the physical density distributions. Although we will make no direct use of this minimization principle here, relying instead on Eq. (6), its importance in providing both a physical picture and an avenue for developing numerical algorithms is not to be underestimated.

### B. The Kohn-Sham equations

The power of DFT stems from the feasibility of finding accurate and simple approximations for the complicated many-body interaction effects in the free energy $F_{\mathrm{HK}}$. Kohn and Sham exploited the fact that the noninteracting effects are much

simpler to deal with and, nevertheless, contain the lion's share of the physics of the full system. To introduce the Kohn-Sham scheme, the first step is to separate the Hohenberg-Kohn free energy into two contributions,

$$F_{\rm HK}([n,\mathbf{m}],T,\Lambda=1)=F_{\rm ni}([n,\mathbf{m}],T)+F_{\rm int}([n,\mathbf{m}],T), \quad (8)$$

where the noninteracting free energy $F_{\rm ni}$ of the Kohn-Sham system is defined as $F_{\rm HK}$ in the absence of interactions (i.e., at $\Lambda=0$), and the term $F_{\rm int}$ is defined as the difference between the full $F_{\rm HK}$ at $\Lambda=1$ and $F_{\rm ni}$ (i.e., it contains all of the complicated interaction effects). In DFT for electrons, it is standard to further separate the interaction term into a simple Hartree long-range interaction term and an exchange-correlation term, which is usually considerably smaller and for which approximations are sought and employed. As will be clarified later, for neutral atoms interacting with short-range potentials, the Hartree (direct) and the exchange contributions are of comparable (often equal) magnitudes, and, therefore, we proceed with lumping the interactions into a single term.

It follows, from Eq. (8), that each of the derivatives in Eq. (6) can also be written as a sum of two terms,

$$\begin{aligned} v_{\rm ext}(\mathbf{r})&=v_{\rm ni}(\mathbf{r})-v_{\rm int}(\mathbf{r}),\\ \mathbf{B}_{\rm ext}(\mathbf{r})&=\mathbf{B}_{\rm ni}(\mathbf{r})-\mathbf{B}_{\rm int}(\mathbf{r}),\end{aligned} \quad (9)$$

where we have used subscripts ext and ni to denote the potentials corresponding to the $[n,\mathbf{m}]$ densities for $\Lambda=1$ and for $\Lambda=0$, respectively, and the interaction potentials are defined as

$$v_{\rm int}(\mathbf{r})=\frac{\delta F_{\rm int}}{\delta n\,(\mathbf{r})},\quad \mathbf{B}_{\rm int}(\mathbf{r})=-\frac{\delta F_{\rm int}}{\delta \mathbf{m}\,(\mathbf{r})}, \quad (10)$$

with a convention for the signs which is opposite that of Eq. (6). The external potentials and/or fields $[v_{\rm ext},\mathbf{B}_{\rm ext}]$ are known *a priori* in standard applications, whereas, the noninteracting potentials $[v_{\rm ni},\mathbf{B}_{\rm ni}]$ (traditionally called effective potentials), which are required to reproduce the same density distributions $[n,\mathbf{m}]$ as in the fully interacting system, but without interactions, are not initially known and must be found. Equation (9) immediately gives

$$\begin{aligned} v_{\rm ni}(\mathbf{r})&=v_{\rm ext}(\mathbf{r})+v_{\rm int}(\mathbf{r}),\\ \mathbf{B}_{\rm ni}(\mathbf{r})&=\mathbf{B}_{\rm ext}(\mathbf{r})+\mathbf{B}_{\rm int}(\mathbf{r}),\end{aligned} \quad (11)$$

which gives the noninteracting or effective potentials in terms of the externally applied fields plus a contribution due to interactions. The system of noninteracting particles in these effective potentials serves as the reference system for DFT calculations—this is the Kohn–Sham system already referred to.

Equation (11) represents a self-consistent requirement, which lies at the heart of the Kohn-Sham scheme: Given an initial guess for the density distributions and a practical approximation for the interaction contribution, this relation specifies the potentials for the noninteracting reference (Kohn-Sham) system. This reference system may be solved using the known tools for noninteracting particles (e.g., the single-particle Schrödinger equation with the Fermi-Dirac distribution for the occupations of the electrons). The new densities may then be used as an improved guess, yielding new values for the noninteracting potentials, in an iterative fashion. The iterations are stopped once self-consistency has been achieved to the desired accuracy.

The approximation to be used for $F_{\rm int}$ remains to be specified. We will limit attention here to LDAs of the type suggested (for electrons) by Kohn and Sham [20]. Within this approach, the interaction term is approximated by using the properties of *uniform* interacting systems:

$$F_{\rm int}\simeq\int d\mathbf{r}\, f_{\rm int}(\mathbf{n}(\mathbf{r}),\mathbf{m}(\mathbf{r})). \quad (12)$$

Here, $f_{\rm int}(n,\mathbf{m})$ is the contribution of interactions to the Hohenberg-Kohn free energy of a uniform system with densities $n$ and $\mathbf{m}$, calculated per unit volume. With this simple expression for the interaction term, the functional derivatives defining the contribution to the potentials, Eq. (10), can easily be taken

$$\begin{aligned} v_{\rm int}(\mathbf{r})&=\frac{\partial f_{\rm int}}{\partial n}\,(n(\mathbf{r}),\mathbf{m}(\mathbf{r})),\\ \mathbf{B}_{\rm int}(\mathbf{r})&=-\frac{\partial f_{\rm int}}{\partial \mathbf{m}}\,(n(\mathbf{r}),\mathbf{m}(\mathbf{r})).\end{aligned} \quad (13)$$

Knowledge of $f_{\rm int}(n,\mathbf{m})$ comes from outside of DFT. The uniform system is much simpler than the nonuniform system in principle, but evaluation of the many-body effects, even in the uniform case, can require sophisticated techniques. For example, for electron systems, quantum Monte Carlo techniques have been employed, as already noted. Once the results are found, the function $f_{\rm int}(n,\mathbf{m})$ can be tabulated or otherwise efficiently represented. Thus, DFT allows one to import the results of sophisticated calculations for uniform systems and to use them as input for the calculations of inhomogeneous systems.

It is of interest to note that the thermodynamic derivation used here is constructive. For example, it immediately gives the exact relation $F_{\rm int}=\int_0^1 d\Lambda\,(\partial F/\partial\Lambda)$ with the integrand $(\partial F/\partial\Lambda)$ equal to $\partial\Omega/\partial\Lambda=\langle\hat{H}_{\rm int}\rangle$, which, in the context of electrons, has been called the adiabatic connection formula [49] and has been derived via a much less direct route. For weakly interacting bosons, it is appropriate to approximate the integrand by its noninteracting value at $\Lambda=0$. As we will see in the following, this yields a particularly simple approximation for $F_{\rm int}$, which is again local [i.e., of the form of Eq. (12)].

## III. DFT FOR BOSONS—Φ-DFT

In this section, a version of DFT adapted to bosonic systems, in which the condensate will be treated as a separate field (the condensate field Φ), in addition to the density, will be developed. A system of identical bosonic atoms of mass $m$ in an external potential $v_{\rm ext}(\mathbf{r})$ can be described, in second-quantized notation, by the Hamiltonian,

$$\hat{H}=\int d\mathbf{r}\,\hat{\psi}^\dagger\left(-\frac{\hbar^2\nabla^2}{2m}+v_{\rm ext}\right)\hat{\psi}+\hat{H}_{\rm int}, \quad (14)$$

where the interaction term involves a two-body interaction potential $V(\mathbf{r}-\mathbf{r}')$. This potential has a hard-core repulsive form at small interatomic separations and a long-range attractive van der Waals form outside the core. As explained in

Sec. I, for a dilute gas, with the typical distance between atoms much larger than the range of the potential, only the $s$-wave scattering contribution is significant, and the interaction can fully be characterized by a single parameter $a_0$, the $s$-wave scattering length.

The scattering length $a_0$ is typically on the order of nanometers, while the typical distance between the atoms $n^{-1/3}$, in experiments, is on the order of hundreds of nanometers. Therefore, one may use a Hamiltonian with a point interaction,

$$\hat{H}_{\rm int} = \frac{g}{2}\int d\mathbf{r}\,\hat{\psi}^\dagger\hat{\psi}^\dagger\hat{\psi}\,\hat{\psi}, \tag{15}$$

where a high-momentum cutoff $\hbar k_c$ is implied (i.e., no attempt to describe the components of the field $\hat{\psi}$ on length scales as small as the range of the interaction potential is made). Note that physical quantities derived from this Hamiltonian depend on both the interaction strength $g$ and the cutoff $k_c$. For example, the $s$-wave scattering length is related to the parameters in the Hamiltonian by $a_0 \simeq gm/4\pi\hbar^2$ only to leading order in $g$, with corrections of order $k_c a_0^2$, which will be assumed small. This undesirable feature may be avoided by using a short-range pseudopotential [45,50], an option that will not be made explicit here but is necessary when large values of $a_0$ are encountered (Feshbach resonances). Note that different forms of $\hat{H}_{\rm int}$ are legitimate within DFT as developed later and are associated with different interaction contributions $F_{\rm int}$. Thus, when the pseudopotential form of $\hat{H}_{\rm int}$ is used and the corresponding changes are made in $F_{\rm int}$, all of the DFT expressions to be derived in the following will remain valid (expressions for $F_{\rm int}$ beyond the leading order are not included in the present paper). Furthermore, one may include, for example, three-body interactions, simply by modifying $F_{\rm int}$ appropriately.

### A. The grand potential and the free energy

For a bosonic system coupled to a particle reservoir at chemical potential $\mu$ and temperature $T$, the grand potential may be written as

$$\Omega([v-\mu,\eta,\eta^*],T,\Lambda) = -k_B T \ln {\rm Tr}\exp\left(-\frac{\hat{H}^{(\mu)}}{k_B T}\right), \tag{16}$$

where the trace is over the full many-body Hilbert space. Fictitious potential fields $\eta(\mathbf{r})$ and $\eta^*(\mathbf{r})$, which break the particle-number conservation symmetry, have been included here in order to couple to the condensate fields $\Phi(\mathbf{r})$ and $\Phi^*(\mathbf{r})$, which will be introduced shortly. The grand-canonical Hamiltonian $\hat{H}^{(\mu)} \equiv \hat{H} - \mu\hat{N}$ with $\hat{N}$ as the number operator, is

$$\hat{H}^{(\mu)} = \int d\mathbf{r}\left\{\hat{\psi}^\dagger\left(-\frac{\hbar^2\nabla^2}{2m} + v - \mu\right)\hat{\psi} - \eta\hat{\psi}^\dagger - \eta^*\hat{\psi}\right\} + \Lambda\hat{H}_{\rm int}. \tag{17}$$

It will be convenient to treat $\eta(\mathbf{r})$ and $\eta^*(\mathbf{r})$ [and, similarly, $\Phi(\mathbf{r})$ and $\Phi^*(\mathbf{r})$, see later] as independent, and to set them equal to the complex conjugates of each other at the end of the calculation. Clearly, the physical fictitious fields vanish, $\eta_{\rm ext}(\mathbf{r}) = \eta^*_{\rm ext}(\mathbf{r}) = 0$, but the noninteracting or effective fields $\eta_{\rm ni}(\mathbf{r}) = \eta_{\rm int}(\mathbf{r})$ may be significant.

The statistical-physics definition of Eq. (16) fulfills all the thermodynamic requirements assumed in Sec. II. Specifically, it follows directly from Eq. (16) that $\Omega$ is concave [51]. Its functional derivatives are as described in Eq. (1), where we can now identify the density as

$$n(\mathbf{r}) = \frac{\delta\Omega}{\delta v(\mathbf{r})} = \langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle, \tag{18}$$

and the condensate field,

$$\Phi(\mathbf{r}) = -\frac{\partial\Omega}{\partial\eta^*(\mathbf{r})} = \langle\hat{\psi}(\mathbf{r})\rangle, \tag{19}$$

with the corresponding expression for $\Phi^*$ implied. The entropy and interaction energy are given by

$$S = -\frac{\partial\Omega}{\partial T}, \qquad \mathcal{E}_{\rm int} = \langle\hat{H}_{\rm int}\rangle = \frac{\partial\Omega}{\partial\Lambda}. \tag{20}$$

The principles of DFT detailed in Sec. II may now be applied, with the fictitious potential and the condensate field replacing the "magnetic" terms $\mathbf{B}(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$. Thus, the Hohenberg-Kohn free energy is

$$F_{\rm HK}([n,\Phi,\Phi^*],T,\Lambda) = \Omega([v-\mu],T,\Lambda) - \int d\mathbf{r}\,\{(v-\mu)n - \eta^*\Phi - \eta\Phi^*\}, \tag{21}$$

and its derivatives are

$$\frac{\delta F_{\rm HK}}{\delta n} = -(v-\mu), \quad \frac{\delta F_{\rm HK}}{\delta\Phi} = \eta^*, \tag{22}$$

$$\frac{\partial F_{\rm HK}}{\partial T} = -S, \quad \frac{\partial F_{\rm HK}}{\partial\Lambda} = \mathcal{E}_{\rm int}. \tag{23}$$

### B. The Kohn-Sham equations

Next, we apply the Kohn-Sham approach, based on the partition in Eq. (8) of $F_{\rm HK}$ into a term describing a noninteracting reference system and an interaction term. The noninteracting reference system (i.e., the Kohn-Sham system) is described by the grand-canonical Hamiltonian (we drop the $\mu$ superscript to simplify notation),

$$\hat{H}_{\rm ni} = \int d\mathbf{r}\left[\hat{\psi}^\dagger\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right)\hat{\psi} - \eta_{\rm ni}\hat{\psi}^\dagger - \eta^*_{\rm ni}\hat{\psi}\right], \tag{24}$$

with the noninteracting (or effective) potentials given by Eq. (11). The field operator $\hat{\psi}(\mathbf{r})$ may be written in terms of the condensate field $\Phi(\mathbf{r})$ and a residual operator field $\hat{\phi}(\mathbf{r})$:

$$\hat{\psi}(\mathbf{r}) = \Phi(\mathbf{r}) + \hat{\phi}(\mathbf{r}). \tag{25}$$

The requirement $\langle\hat{\phi}(\mathbf{r})\rangle = 0$, cf. Eq. (19), is associated with a modified G-P equation,

$$\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right)\Phi = \eta_{\rm ni}. \tag{26}$$

This condition leads to the vanishing of the linear-in-$\hat{\phi}^\dagger$ (and, similarly, in $\hat{\phi}$) terms in the Hamiltonian,

$$\hat{H}_{\rm ni} = \hat{H}_{\rm th} + \hat{H}_{\rm con} = \int d\mathbf{r} \left[ \hat{\phi}^\dagger \left( -\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu \right) \hat{\phi} - \frac{1}{2}(\eta_{\rm ni}\Phi^* + \eta_{\rm ni}^*\Phi) \right], \quad (27)$$

and, hence, to $\langle\hat{\phi}(\mathbf{r})\rangle = 0$. A partial cancellation of the term involving the condensate field has occurred here, and we have introduced notation separating thermal and condensate parts.

The Schrödinger equation associated with the thermal part of the Hamiltonian is

$$\left( -\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu \right) \varphi_j = \varepsilon_j \varphi_j \quad (28)$$

for the single-particle wave functions $\varphi_j$ and their eigenvalues $\varepsilon_j$ (i.e., the single-particle energies measured from the chemical potential). Using eigenstate creation and annihilation operators,

$$\hat{\phi}(\mathbf{r}) = \sum_j \varphi_j(\mathbf{r})\hat{a}_j, \quad \hat{\phi}^\dagger(\mathbf{r}) = \sum_j \varphi_j^*(\mathbf{r})\hat{a}_j^\dagger, \quad (29)$$

one may rewrite this effective noninteracting many-body Hamiltonian as

$$\hat{H}_{\rm th} = \sum_j \varepsilon_j \hat{a}_j^\dagger \hat{a}_j. \quad (30)$$

Then, it becomes straightforward to evaluate the statistical-mechanical properties of this noninteracting Kohn-Sham system. The grand potential, Eq. (16), also separates into two parts,

$$\Omega_{\rm ni}([v_{\rm ni}-\mu,\eta_{\rm ni},\eta_{\rm ni}^*],T) = \Omega_{\rm th}([v_{\rm ni}-\mu],T) + \Omega_{\rm con}([v_{\rm ni}-\mu,\eta_{\rm ni},\eta_{\rm ni}^*]), \quad (31)$$

where

$$\Omega_{\rm th}([v_{\rm ni}-\mu],T) = k_B T \sum_j \ln\left[ 1 - \exp\left( -\frac{\varepsilon_j}{k_B T} \right) \right] \quad (32)$$

(the requirement that the chemical potential be lower than the ground state of the Schrödinger equation $\min_j \varepsilon_j > 0$ is manifest here), and

$$\Omega_{\rm con}([v_{\rm ni}-\mu,\eta_{\rm ni},\eta_{\rm ni}^*]) = -\frac{1}{2}\int d\mathbf{r}\,(\eta_{\rm ni}\Phi^* + \eta_{\rm ni}^*\Phi). \quad (33)$$

The Schrödinger equation, Eq. (28), determines the eigenvalues in $\Omega_{\rm th}$, and the Kohn-Sham form of the G-P equation, Eq. (26), determines the condensate field in $\Omega_{\rm con}$. Note that the effective noninteracting potential $v_{\rm ni}$ appears in both, whereas the fictitious potential $\eta_{\rm ni}$ appears only in the latter, and that $\Omega_{\rm con}$ does not depend on the temperature $T$.

Turning to the functional derivatives, one finds that the density distribution, Eq. (18), becomes

$$n(\mathbf{r}) = n_{\rm th}(\mathbf{r}) + n_{\rm con}(\mathbf{r}) = \sum_j \frac{|\varphi_j(\mathbf{r})|^2}{\exp(\varepsilon_j/T) - 1} + \Phi^*(\mathbf{r})\Phi(\mathbf{r}), \quad (34)$$

together with $\Phi = -\delta\Omega_{\rm con}/\delta\eta_{\rm ni}^*$. These relations not only are obvious from Eq. (25), but also can be derived from Eq. (26). Explicitly, one takes its variation and multiplies by $\Phi^*$ to obtain

$$\Phi^* \left( -\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu \right) \delta\Phi + \Phi^*\Phi\,\delta v_{\rm ni} = \Phi^*\,\delta\eta_{\rm ni}, \quad (35)$$

where the first term may be identified as $\eta_{\rm ni}^*\,\delta\Phi$, and

$$\delta\Omega_{\rm con} = \int d\mathbf{r}\,(-\Phi^*\,\delta\eta_{\rm ni} - \Phi\,\delta\eta_{\rm ni}^* + \Phi^*\Phi\,\delta v_{\rm ni}) \quad (36)$$

follows.

The Hohenberg-Kohn free energy is

$$F_{\rm ni}([n,\Phi,\Phi^*],T) = F_{\rm th}([n-\Phi^*\Phi],T) + F_{\rm con}[\Phi,\Phi^*], \quad (37)$$

with

$$F_{\rm th}([n_{\rm th}],T) = k_B T \sum_j \ln\left[ 1 - \exp\left( -\frac{\varepsilon_j}{k_B T} \right) \right] - \int d\mathbf{r}\, n_{\rm th}(v_{\rm ni} - \mu), \quad (38)$$

and

$$F_{\rm con}[\Phi,\Phi^*] = \int d\mathbf{r}\,\Phi^* \left( -\frac{\hbar^2\nabla^2}{2m} \right) \Phi. \quad (39)$$

As is generally the case with Legendre transforms, the RHS of Eq. (38) is evaluated at the potential $v_{\rm ni}(\mathbf{r})$ which corresponds to the given density $n_{\rm th}(\mathbf{r})$, and it is difficult to make it more explicit. However, use of Eq. (26) has yielded a significant simplification in the condensate term, defined as $F_{\rm con} = \Omega_{\rm con} - \int d\mathbf{r}\,[(v_{\rm ni}-\mu)n_{\rm con} - \eta_{\rm ni}\Phi^* - \eta_{\rm ni}^*\Phi]$, resulting in the explicit form of Eq. (39). The rule for Legendre transforms of sums, such as $\Omega_{\rm ni} = \Omega_{\rm th} + \Omega_{\rm con}$, is that each term can be transformed separately, $\Omega_{\rm th}$ into $F_{\rm th}$ and $\Omega_{\rm con}$ into $F_{\rm con}$, but the sum must be evaluated as $F_{\rm ni}[n] = F_{\rm th}[n_{\rm th}] + F_{\rm con}[n_{\rm con}]$ with the conditions $n = n_{\rm th} + n_{\rm con}$ and $\delta F_{\rm th}/\delta n_{\rm th} = \delta F_{\rm con}/\delta n_{\rm con}$ implied. In the present case, the contribution of the condensate to the density $n_{\rm con} = \Phi^*\Phi$ is known in terms of the condensate amplitude, which is itself a free variable, and no implicit relationship remains to be evaluated. In other words, the fact that $\delta\Omega_{\rm con}/\delta v_{\rm ni} = \Phi^*\Phi$ is trivially related to $\delta\Omega_{\rm con}/\delta\eta_{\rm ni}^* = -\Phi$ plays a significant simplifying role, resulting in $F_{\rm con}$ depending only on $\Phi$ and $\Phi^*$ and $F_{\rm th}$ depending only on $n - \Phi^*\Phi$.

To summarize, the Kohn-Sham equations for a system of bosons are Eq. (26) for the condensate field, Eqs. (28) and (34) for the density, and $v_{\rm ni} = v_{\rm ext} + v_{\rm int}$ and $\eta_{\rm ni} = \eta_{\rm int}$ for the effective potentials from Eq. (11). For an LDA, we have

$$v_{\rm int} = \partial f_{\rm int}/\partial n, \quad \eta_{\rm int} = -\partial f_{\rm int}/\partial\Phi^*, \quad (40)$$

where specific expressions for the interaction energy density $f_{\rm int}(n,\Phi,\Phi^*)$ will be suggested in the following. Once these Kohn-Sham equations have been solved, the grand potential

may be evaluated as

$$\Omega = \Omega_{\rm ni} + F_{\rm int} - \int d\mathbf{r}\,[(v_{\rm ni} - v_{\rm ext})n - (\eta_{\rm ni}\Phi^* + \eta_{\rm ni}^*\Phi)]$$
$$= \sum_j k_B T\,\ln\left[1 - \exp\left(-\frac{\varepsilon_j}{k_B T}\right)\right]$$
$$+ \int d\mathbf{r}\left[(f_{\rm int} - n v_{\rm int}) + \frac{1}{2}(\eta_{\rm int}\Phi^* + \eta_{\rm int}^*\Phi)\right]. \quad (41)$$

Here, the integral is a generalized subtraction of the double counting of the interaction energy included in the single-particle energies, as customarily occurs in Hartree-like schemes.

Note that, for fermions, there is no condensate term, and, in the low-temperature limit, $F_{\rm ni}$ is simply the kinetic energy $K$. The temperature and entropy can be thought of as a correction that is necessary at finite temperatures. For noninteracting bosons, one still has $F_{\rm th} = K + TS$, but both terms vanish as the temperature is lowered, and for large condensates, the zero-point kinetic energy $F_{\rm con}$ also may be negligible. In such cases, one has no significant contribution to the Hohenberg-Kohn free energy from the Kohn-Sham system and $F \simeq F_{\rm int}$ in the low-temperature limit.

### 1. The Thomas-Fermi approximation

Many of the relevant BEC systems studied experimentally involve a large number of bosonic atoms, in the thousands or millions, in a smooth external potential. In such cases, it is appropriate to introduce the Thomas-Fermi approximation [15] (adapted from many electron systems), which takes the density of single-particle states in phase space to be $(2\pi\hbar)^{-3}$ and uses the classical relationship $\varepsilon = \frac{p^2}{2m} + v_{\rm ni}(\mathbf{r}) - \mu$. Thus, the local density of states is approximated as

$$d(\varepsilon,\mathbf{r}) = \int_0^\infty \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\delta\left(\varepsilon - \frac{|\mathbf{p}|^2}{2m} - v_{\rm ni}(\mathbf{r}) + \mu\right)$$
$$= \Theta[\varepsilon - v_{\rm ni}(\mathbf{r}) + \mu]\frac{m\sqrt{2m[\varepsilon - v_{\rm ni}(\mathbf{r}) + \mu]}}{2\pi^2\hbar^3}, \quad (42)$$

and the overall density of states is given by

$$d(\varepsilon) = \sum_j \delta(\varepsilon - \varepsilon_j) = \int d\mathbf{r}\, d(\varepsilon,\mathbf{r}). \quad (43)$$

With this approximation, there is no need to solve the Schrödinger equation, Eq. (28), which is the step that is most significant in terms of computational resources. Expressions, such as Eqs. (32) and (34), are then evaluated as simple integrals over the corresponding density of states, Eqs. (43) or (42), respectively. For example, the noninteracting grand potential, from Eqs. (32) and (43), becomes

$$\Omega_{\rm th} = k_B T \lambda_T^{-3}\int d\mathbf{r}\, f\left(\frac{v_{\rm ni} - \mu}{k_B T}\right), \quad (44)$$

where $\lambda_T$ is the thermal de Broglie wavelength mentioned in Sec. I, and

$$f(x) = \frac{4}{\sqrt{\pi}}\int_0^\infty q^2\,dq\,\ln(1 - e^{-q^2 - x}) = -\sum_{l=1}^\infty \frac{e^{-lx}}{l^{5/2}}, \quad (45)$$

with $x = (v_{\rm ni} - \mu)/k_B T$ and $q$ is a scaled momentum variable. The function $f(x)$ is known as the *polylogarithm* or *de Jonquiere's function* and is plotted in Fig. 2. It varies from $-\zeta(5/2)$ to 0 as $x$ is varied from 0 to $\infty$ [the Riemann $\zeta$ function evaluates to $\zeta(5/2) = 1.341,\ldots$]. Its derivative (also plotted), which varies from $\zeta(3/2) = 2.612,\ldots$ to 0, determines the density,

$$n_{\rm th}(\mathbf{r}) = \lambda_T^{-3} f'\left(\frac{v_{\rm ni} - \mu}{k_B T}\right). \quad (46)$$

Its Legendre transform (cf. the figure again) is

$$\tilde{f}(u) = \max_x\{f(x) - ux\}, \quad (47)$$

with $u = \lambda_T^3 n_{\rm th}$, the dimensionless density, and this determines the noninteracting Hohenberg-Kohn free energy as

$$F_{\rm th}([n_{\rm th}],T) = k_B T\lambda_T^{-3}\int d\mathbf{r}\,\tilde{f}(\lambda_T^3 n_{\rm th}). \quad (48)$$

The Thomas-Fermi approximation is appropriate for systems with gradual inhomogeneities. It may be applied to the condensate component as well, by simply dropping the gradient term in Eq. (26), which amounts to neglecting the zero-point energy of the condensate $F_{\rm con} \simeq 0$ [this corresponds

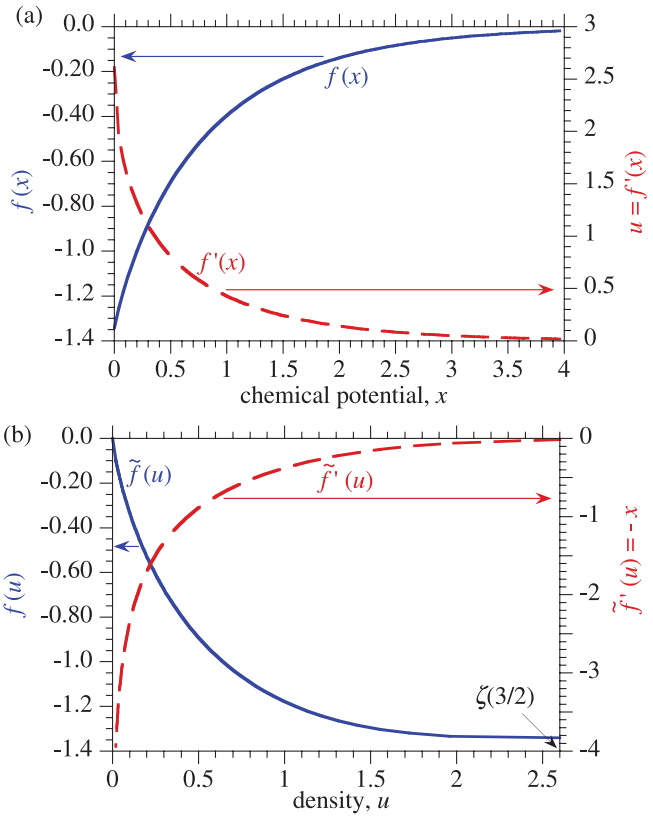


FIG. 2. (Color online) Relationships for the thermal components according to the Thomas-Fermi approximation: $f$ is the scaled grand potential, $x$ is the scaled effective potential, $u$ is the scaled density, and $\tilde{f}$ is the scaled Hohenberg-Kohn free energy. (a) The function $f(x)$ (full line) and its derivative $u(x)$ (dotted line). (b) The Legendre transform $\tilde{f}(u)$ (full line) and its derivative $-x(u)$ (dotted line). Note that the derivatives are simply inverse functions.

to $\Omega_{\rm con} \simeq \int d\mathbf{r}\,(v_{\rm ni}-\mu)\Phi^*\Phi$ in the present notation]. As mentioned in Sec. I, when all the finite-size effects due to the inhomogeneities in the system are indeed negligible, it is appropriate to use a local-equilibrium approach with the density $n(\mathbf{r})$ at each position taken as that, which, for an infinite system, would correspond to the given local value of the chemical potential $\mu - v_{\rm ext}(\mathbf{r})$. Applications of DFT for such situations approach the local-equilibrium results. For $\Phi$-DFT, the condensate amplitude $\Phi(\mathbf{r})$ relaxes to the value corresponding to an infinite system of density $n(\mathbf{r})$, and, thus, there is no point in including it as a separate functional variable.

### C. Interaction effects

In order to complete the DFT description, an approximate description of the interaction term $F_{\rm int}([n,\Phi,\Phi^*],T)$ must be specified. As noted at the end of Sec. II, the simplest approximation is obtained by equating the integrand in the adiabatic connection formula with its value for noninteracting bosons,

$$F_{\rm int}([n,\Phi,\Phi^*],T) \simeq \int d\mathbf{r}\,\frac{g}{2}[2n^2-(\Phi^*\Phi)^2], \qquad (49)$$

or $f_{\rm int} = (g/2)[2n^2-(\Phi^*\Phi)^2]$ in the notation of Eq. (12). The factor of 2 in the brackets comes from counting both the direct and the exchange contributions, and the subtraction comes from the fact that exchange is not relevant to the condensate's interaction with itself. From Eq. (40), this leads to

$$v_{\rm int} = 2gn, \quad \eta_{\rm int} = g(\Phi^*\Phi)\Phi, \qquad (50)$$

or to

$$v_{\rm ni} = v_{\rm ext} + 2gn, \quad \eta_{\rm ni} = g(\Phi^*\Phi)\Phi. \qquad (51)$$

Using the latter in Eq. (26) gives the G-P equation,

$$\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ext} - \mu + 2gn_{\rm th} + g\Phi^*\Phi\right)\Phi = 0. \qquad (52)$$

As mentioned in Sec. I, here, the interaction terms differ from the simple $2gn$ appearing in the effective potential due to the absence of an exchange contribution to the condensate-condensate interactions. The first-order approximation of Eq. (49), with $f_{\rm int}$ quadratic in $n$, $\Phi$, and $\Phi^*$, leads to simplification of Eq. (41) for the grand potential, resulting in $\Omega = \Omega_{\rm th} - \int f_{\rm int}\,d\mathbf{r}$, where the subtraction of the double counting of the interaction energy is explicit. This simplification is not as dramatic as it may seem, as the subtraction can only be evaluated after the Kohn-Sham system of equations has been solved (either with or without the Thomas-Fermi approximation for the thermal cloud and for the condensate).

Note that Eq. (52) is identical to the G-P equation derived from the field-theory approach in the Popov approximation [44]. The present level of description, with the Thomas-Fermi approximation for the density of the thermal component, Eq. (46), reproduces the two-fluid description of finite-temperature BECs [41] mentioned in Sec. I. The present $\Phi$-DFT provides a route for improvements in this description, based on improved evaluations of $f_{\rm int}(n,\Phi,\Phi^*,T)$. In fact, we will see, in Sec. V, that such improvements can be appreciable even when the interactions are not particularly strong. Furthermore, $\Phi$-DFT allows treatment of systems with significant inhomogeneities, which are not describable by the simple two-fluid equations.

Before closing this section, it is appropriate to describe the differences in treatment which are obtained for a DFT of bosons with only a single density. At zero temperature, one has $n_{\rm th} = 0$ or $n = \Phi^*\Phi$, a single-density treatment would have $f_{\rm int}(n) = gn^2/2$, and the G-P equation [Eq. (52) without $n_{\rm th}$] arises as the ground-state solution of the Schrödinger equation and need not be derived by shifting the quantum operator as in Eq. (26). Thus, in this limit, the present treatment does not differ significantly from the single-density DFT treatment suggested by Nunes [37]. Substantial differences do arise at finite temperatures, where a single-density treatment with a first-order local approximation would have $f_{\rm int} = (g/2)\{2n^2 - [n-\zeta(3/2)\lambda_T^{-3}]^2\}$, and the corresponding effective potential $v_{\rm eff} = v_{\rm ext} + g(n+n_{\rm th})$ with $n_{\rm th} = \zeta(3/2)\lambda_T^{-3}$ would still give rise to an equation for the ground state, which is essentially the correct G-P equation, but the excited states would be subject to the wrong potential. In the limit of weak inhomogeneities, the situation can be remedied. The Thomas-Fermi approximation holds with $v_{\rm ni}-\mu = 0$ at points with a condensate [i.e., with $n > \zeta(3/2)\lambda_T^{-3}$]. The corresponding free-energy function is $\tilde{f}(u)$ with $u = \lambda_T^3 n$ and is to be continued for large densities $u > \zeta(3/2)$. According to the rules for Legendre transforms, Eq. (47), it is simply linear in this regime. The solution of the Kohn-Sham system of equations for points with $v_{\rm ni}(\mathbf{r}) = \mu$ would then seem to be ambiguous, as there is a range of densities for a single value of the effective potential, but the condition $v_{\rm ext}(\mathbf{r}) + v_{\rm int}(n(\mathbf{r})) = \mu$ may be used to determine the density $n(\mathbf{r})$ instead. If the interaction energy $f_{\rm int}(n)$ correctly accounts for the difference between the reference system and the interacting system, then the correct results for the free energy and the density distribution are guaranteed to be obtained. It is only in the presence of significant inhomogeneities that the weakness of this approach (i.e., the effect of its having essentially the same potential in the Schrödinger and the G-P equations) will show up.

## IV. DFT FOR BOSONS WITH ANOMALOUS TERMS—A-DFT

In this section, the thermodynamic approach will be used to develop another version of DFT for bosonic systems, which results from adding a term of the form $-\int d\mathbf{r}\,[\xi\hat{\psi}^\dagger\hat{\psi}^\dagger + \xi^*\hat{\psi}\hat{\psi}]$ to the Hamiltonian. Here, $\xi(\mathbf{r})$ is a second fictitious potential—an anomalous potential—which is to be set equal to zero in the fully interacting system $\xi_{\rm ext} = 0$. The fact that it does not vanish in the Kohn-Sham reference system $\xi_{\rm ni} \neq 0$ will result in a level of treatment generalizing that of Bogoliubov. In order to assist the reader, here, the partitioning into subsections is precisely parallel to that of Sec. III presenting $\Phi$-DFT.

### A. The grand potential and the free energy

The thermodynamic treatment of the enlarged Hamiltonian follows the same steps as earlier, with Eq. (16) defining the grand potential, which acquires a $[\xi,\xi^*]$ dependence. The corresponding derivative is

$$\Delta(\mathbf{r}) = -\frac{\delta\Omega}{\delta\xi^*(\mathbf{r})} = \langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\rangle, \qquad (53)$$

where $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$ as well as $\eta(\mathbf{r})$ and $\eta^*(\mathbf{r})$ play the role of $\mathbf{B}(\mathbf{r})$. The Legendre transform leading to the Hohenberg-Kohn free energy is

$$F_{\rm HK}([n,\Phi,\Phi^*,\Delta,\Delta^*],T,\Lambda) = \Omega([v-\mu,\eta,\eta^*,\xi,\xi^*],T,\Lambda) - \int d\mathbf{r}\,[(v-\mu)n - \eta\Phi^* - \eta^*\Phi - \xi\Delta^* - \xi^*\Delta], \quad (54)$$

and we have the additional relation

$$\frac{\delta F_{\rm HK}}{\delta\Delta} = \xi^*. \quad (55)$$

### B. The Bogoliubov Kohn-Sham system

Here, the Kohn-Sham reference system is described by the noninteracting Hamiltonian,

$$\hat{H}_{\rm ni} = \int d\mathbf{r}\,\hat{\psi}^\dagger\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right)\hat{\psi} - \int d\mathbf{r}\,\{\eta_{\rm ni}\hat{\psi}^\dagger + \eta_{\rm ni}^*\hat{\psi} + \xi_{\rm ni}\hat{\psi}^\dagger\hat{\psi}^\dagger + \xi_{\rm ni}^*\hat{\psi}\hat{\psi}\}, \quad (56)$$

where the noninteracting effective potential $v_{\rm ni}$ and auxiliary fields $\eta_{\rm ni}, \xi_{\rm ni}$ are again to be defined by Eq. (11) and determined by the interactions. Shifting the field operator by a scalar as in Eq. (25), $\hat{\psi}(\mathbf{r}) = \Phi(\mathbf{r}) + \hat{\phi}(\mathbf{r})$ and requiring all terms linear in the operators $\hat{\phi}^\dagger$ (and $\hat{\phi}$) to cancel from the Hamiltonian, yields, in this case,

$$\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right)\Phi - \eta_{\rm ni} - 2\xi_{\rm ni}\Phi^* = 0. \quad (57)$$

The Kohn-Sham Hamiltonian becomes

$$\hat{H}_{\rm ni} = \hat{H}_{\rm nc} + \hat{H}_{\rm con}, \quad (58)$$

with

$$\hat{H}_{\rm nc} = \int d\mathbf{r}\,\left\{\hat{\phi}^\dagger\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right)\hat{\phi} - \xi_{\rm ni}\hat{\phi}^\dagger\hat{\phi}^\dagger - \xi_{\rm ni}^*\hat{\phi}\hat{\phi}\right\}, \quad (59)$$

and $\hat{H}_{\rm con} = -\frac{1}{2}\int d\mathbf{r}\,(\eta_{\rm ni}\Phi^* + \eta_{\rm ni}^*\Phi)$ as before, Eq. (27). The subscript nc represents the noncondensed part of the boson system, which persists at zero temperature and, thus, should not be referred to as a thermal component. Note the complete cancellation of terms of type $\int d\mathbf{r}\,\xi_{\rm ni}^*\Phi^2$ in the effective Hamiltonian—the contributions from $\Phi^*(\cdots)\Phi$and $\xi_{\rm ni}^*\Phi^2$ are equal and opposite due to Eq. (57). In contrast, the terms of type $\int d\mathbf{r}\,\eta_{\rm ni}\Phi^*$ only partially cancel, leading to the $\frac{1}{2}$ prefactor in $\hat{H}_{\rm con}$.

The Hamiltonian $\hat{H}_{\rm nc}$ is quadratic in the field operators but does not conserve particle number. This form of Hamiltonian is diagonalized by the Bogoliubov transformation [52]. Following Fetter's notation [53], the field operators may be written as

$$\hat{\phi}(\mathbf{r}) = \sum_j{}' u_j(\mathbf{r})\hat{\gamma}_j - v_j^*(\mathbf{r})\hat{\gamma}_j^\dagger, \quad (60)$$

and its Hermitian conjugate, where the primed sum runs only over positive energy solutions $\mathcal{E}_j > 0$. The $\gamma_j^\dagger$ and $\gamma_j$ are bosonic creation and annihilation operators for the Bogoliubov excitations of the system. The generalized Schrödinger equation for the $(u_j, v_j)$ wave functions is given by

$$\begin{aligned}\left[-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right]u_j - 2\xi_{\rm ni}v_j &= \mathcal{E}_j u_j,\\ \left[-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ni} - \mu\right]v_j - 2\xi_{\rm ni}^*u_j &= -\mathcal{E}_j v_j.\end{aligned} \quad (61)$$

This two-component system of equations, known as the Bogoliubov–de Gennes equation [53], is of the type $\mathcal{H}\binom{u}{v} = \mathcal{E}\sigma_z\binom{u}{v}$ where $\mathcal{H}$ is a Hermitian matrix differential operator, with inner product $\int d\mathbf{r}\,(u_i^*\ v_i^*)\sigma_z\binom{u_j}{v_j} = \int d\mathbf{r}\,(u_i^*u_j - v_i^*v_j)$ involving the Pauli matrix $\sigma_z = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$. The normalization is $\int d\mathbf{r}\,(|u_j|^2 - |v_j|^2) = 1$, and the orthogonality conditions are $\int d\mathbf{r}\,(u_i^*u_j - v_i^*v_j) = 0$ for $i \neq j$ and $\int d\mathbf{r}\,(u_i^*v_j^* - v_i^*u_j^*) = 0$ for all $i$ and $j$ with $\mathcal{E}_i, \mathcal{E}_j > 0$ [54].

Substituting Eq. (60) into Eq. (59), the Hamiltonian becomes

$$\hat{H}_{\rm nc} = \sum_j \mathcal{E}_j\left(\hat{\gamma}_j^\dagger\hat{\gamma}_j - \int d\mathbf{r}\,|v_j|^2\right), \quad (62)$$

which is now in the form of a simple harmonic oscillator for each excitation mode $j$. With Eq. (62), expectation values of different quantities at a temperature $T$ can be evaluated, using either Eq. (60) with $\langle\hat{\gamma}_j\rangle = \langle\hat{\gamma}_j^\dagger\rangle = 0$ and $\langle\hat{\gamma}_i^\dagger\hat{\gamma}_j\rangle = \delta_{ij}\,[\exp(\mathcal{E}_j/T) - 1]^{-1}$, etc., or by explicitly calculating the partition function and the grand potential and taking its derivatives. One finds that $\langle\hat{\psi}(\mathbf{r})\rangle = \Phi(\mathbf{r})$; the density is $n(\mathbf{r}) = n_{\rm nc}(\mathbf{r}) + \Phi^*\Phi$, with

$$n_{\rm nc}(\mathbf{r}) = \langle\hat{\phi}^\dagger\hat{\phi}\rangle = \sum_j\left(\frac{|u_j|^2 + |v_j|^2}{\exp(\mathcal{E}_j/k_BT) - 1} + |v_j|^2\right), \quad (63)$$

and the anomalous density is $\Delta(\mathbf{r}) = \Delta_{\rm nc}(\mathbf{r}) + \Phi^2$, with

$$\Delta_{\rm nc}(\mathbf{r}) = \langle\hat{\phi}\hat{\phi}\rangle = -\sum_j u_j v_j^*\left(\frac{2}{\exp(\mathcal{E}_j/k_BT) - 1} + 1\right). \quad (64)$$

The grand potential of the Kohn-Sham system is $\Omega_{\rm ni} = \Omega_{\rm nc} + \Omega_{\rm con}$, with

$$\Omega_{\rm nc}([v_{\rm ni} - \mu, \xi_{\rm ni}, \xi_{\rm ni}^*], T) = \sum_j\left\{k_BT\ \ln\left[1 - \exp\left(-\frac{\mathcal{E}_j}{k_BT}\right)\right] - \mathcal{E}_j\int d\mathbf{r}\,|v_j|^2\right\}, \quad (65)$$

and $\Omega_{\rm con}[v_{\rm ni} - \mu, \eta_{\rm ni}, \eta_{\rm ni}^*, \xi_{\rm ni}, \xi_{\rm ni}^*] = -\frac{1}{2}\int d\mathbf{r}\,(\eta_{\rm ni}\Phi^* + \eta_{\rm ni}^*\Phi)$ as in Eq. (33). The Hohenberg-Kohn free energy, according to Eqs. (54) and (57), is $F_{\rm ni} = F_{\rm nc} + F_{\rm con}$, with

$$F_{\rm nc}([n - \Phi^*\Phi, \Delta - \Phi^2, \Delta^* - \Phi^{*2}], T) = \sum_j\left(k_BT\ \ln[1 - \exp(-\mathcal{E}_j/k_BT)] - \mathcal{E}_j\int d\mathbf{r}\,|v_j|^2\right) - \int d\mathbf{r}\,[n_{\rm nc}(v_{\rm ni} - \mu) - \Delta_{\rm nc}\xi_{\rm ni}^* - \Delta_{\rm nc}^*\xi_{\rm ni}], \quad (66)$$

and $F_{\rm con}[\Phi,\Phi^*] = \int d\mathbf{r}\, \Phi^*(-\frac{\hbar^2\nabla^2}{2m})\Phi$ as in Eq. (39). The RHS of Eq. (66) is evaluated, as before, with the potentials $v_{\rm ni}$, $\xi_{\rm ni}$, and $\xi^*_{\rm eff}$, which reproduce the noncondensate parts of the density and the anomalous density, through Eqs. (61), (63), and (64). Notice that the noncondensate contribution to each of the thermodynamic quantities $\Omega$, $n$, $\Delta$, and $F$ can be further divided into a temperature-dependent thermal part and an athermal part [e.g., $\Omega_{\rm nc} = \Omega_{\rm th} + \Omega_{\rm ath}$ in Eq. (65)]. The temperature dependence yields an exponential convergence of the thermal parts, and only the athermal parts substantially depend on the cutoff $k_c$ (the above-mentioned rule for the evaluation of a Legendre transform of a sum of two functions applies for $F_{\rm nc} = F_{\rm th} + F_{\rm ath}$, with the requirements $\delta F_{\rm th}/\delta n_{\rm th} = \delta F_{\rm ath}/\delta n_{\rm ath}$ and $n_{\rm th} + n_{\rm ath} = n_{\rm nc}$ implied).

To summarize, the Kohn-Sham equations of A-DFT are Eq. (57) for the condensate amplitude and Eq. (61) for the noncondensate eigenstates and eigenvalues, together with the corresponding expressions for the density and the anomalous density, Eqs. (63) and (64), and together with the self-consistent determination of the effective potentials through Eqs. (11) and (10). The interaction contribution to these potentials will be made explicit in the following. Once this system of equations has been solved, one may use the results to obtain the grand potential for the interacting system, which evaluates as

$$\Omega = \Omega_{\rm nc} + \int d\mathbf{r}\{f_{\rm int} - n v_{\rm int} + \Delta\xi^*_{\rm int} + \Delta^*\xi_{\rm int} + (\eta_{\rm int}\Phi^* + \eta^*_{\rm int}\Phi)/2\}, \tag{67}$$

in full analogy with Eq. (41) of $\Phi$-DFT.

### 1. *Thomas-Fermi approximation for A-DFT*

For applications involving a large number of bosons, a Thomas-Fermi type of approximation can be formulated in the presence of the anomalous potential as well. It is convenient to refer to a momentum variable $\mathbf{p} = \hbar\mathbf{k}$, with the density of states in the single-particle phase space taken as $(2\pi\hbar)^{-3}$, as earlier. The corresponding local-approximation wave function $(u_{\mathbf{k}}, v_{\mathbf{k}})\, \exp(i\mathbf{k}\cdot\mathbf{r})$ consists of plane waves with a bare energy of $\varepsilon_{\mathbf{k}}(\mathbf{r}) = (\hbar^2k^2/2m) + v_{\rm ni}(\mathbf{r}) - \mu$ (including the position dependence due to the effective potential). Equation (61) then takes the form

$$\begin{pmatrix} \varepsilon_{\mathbf{k}} & -2\xi_{\rm ni} \\ -2\xi^*_{\rm ni} & \varepsilon_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \mathcal{E}_{\mathbf{k}}\sigma_z\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}, \tag{68}$$

with the appropriate continuum normalization $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$. Solving this eigensystem of equations gives

$$u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}},$$
$$v_{\mathbf{k}} = (\xi^*_{\rm ni}/|\xi_{\rm ni}|)\, \sinh\theta_{\mathbf{k}},$$
$$\mathcal{E}_{\mathbf{k}} = \varepsilon_{\mathbf{k}}/\cosh 2\theta_{\mathbf{k}} = \sqrt{\varepsilon^2_{\mathbf{k}} - 4|\xi_{\rm ni}|^2}, \tag{69}$$

where $\tanh 2\theta_{\mathbf{k}} = 2|\xi_{\rm ni}|/\varepsilon_{\mathbf{k}}$.

When the noncondensate parts of the thermodynamic quantities are expressed in terms of the solutions of the Bogoliubov–de Gennes equation, they naturally have thermal and athermal parts, as in Eqs. (63)–(65). Here, it will be convenient to introduce dimensionless functions $f_{\rm th}$ and $f_{\rm ath}$ for the corresponding contributions to the grand potential within the Thomas-Fermi approximation,

$$\Omega_{\rm nc} \simeq k_BT\lambda_T^{-3}\int d\mathbf{r}\, f_{\rm th}\left(\frac{v_{\rm ni}-\mu}{k_BT}, \frac{|\xi_{\rm ni}|}{k_BT}\right) + \mathcal{E}_c k_c^3 \int d\mathbf{r}\, f_{\rm ath}\left(\frac{v_{\rm ni}-\mu}{\mathcal{E}_c}, \frac{|\xi_{\rm ni}|}{\mathcal{E}_c}\right), \tag{70}$$

where $\mathcal{E}_c = \hbar^2k_c^2/2m$ is the cutoff energy, $|\xi_{\rm ni}|$ is used as shorthand for $\sqrt{\xi^*_{\rm ni}\xi_{\rm ni}}$, and the functions are defined as

$$f_{\rm th}(x,y) = \frac{4}{\sqrt{\pi}}\int q^2\, dq\, \ln\{1 - \exp[-\sqrt{(q^2+x)^2 - 4y^2}]\}, \tag{71}$$

and

$$f_{\rm ath}(\bar{x},\bar{y}) = \frac{2}{\sqrt{\pi}}\int_0^1 \bar{q}^2\, d\bar{q}\, (\sqrt{(\bar{q}^2+\bar{x})^2 - 4\bar{y}^2} - \bar{q}^2 - \bar{x}) \tag{72}$$

[the notation $x$, $y$, $\bar{x}$, and $\bar{y}$ will be used later as shorthand for the corresponding combinations in Eq. (70)]. Thus, the grand potential of the Kohn-Sham system is the sum of three terms, a condensate part, a thermal part, and an athermal part. As the integral of the athermal part is divergent, we have used the cutoff scale to express it in dimensionless terms (the cutoff dependence of the thermal part is exponentially small and has been ignored). The cutoff energy is large, and it will be appropriate to expand $f_{\rm ath}$ for small values of its variables—see the Appendix. In contrast, the temperature may be small, and so, the whole range of $f_{\rm th}$ will be relevant, except in specific cases, such as at $T = 0$.

The square root in the integrand of Eqs. (71) and (72) is the normalized energy $\mathcal{E}_{\mathbf{k}}$, and for $x = 2y$ or $v_{\rm ni} - \mu = 2|\xi_{\rm ni}|$, it has a linear dependence at small wavenumbers. This represents the phonon branch of the excitation spectrum of the superfluid. The present description also allows for situations with $x > 2y$, which possess a gap in the spectrum at $\mathbf{k} = \mathbf{0}$. As will be discussed further in the following, this gap is not physical.

The Thomas-Fermi results for the density and the anomalous density are

$$n_{\rm nc}(\mathbf{r}) \simeq \lambda_T^{-3}u_{\rm th}(x,y) + k_c^3 u_{\rm ath}(\bar{x},\bar{y}),$$
$$\Delta_{\rm nc}(\mathbf{r}) \simeq \frac{1}{2}\sqrt{\frac{\xi_{\rm ni}}{\xi^*_{\rm ni}}}\left[\lambda_T^{-3}w_{\rm th}(x,y) + k_c^3 w_{\rm ath}(\bar{x},\bar{y})\right], \tag{73}$$

with the following notation for the derivatives:

$$u_{\rm th}(x,y) = \frac{\partial f_{\rm th}(x,y)}{\partial x}, \quad u_{\rm ath}(\bar{x},\bar{y}) = \frac{\partial f_{\rm ath}(\bar{x},\bar{y})}{\partial \bar{x}},$$
$$w_{\rm th}(x,y) = -\frac{\partial f_{\rm th}(x,y)}{\partial y}, \quad w_{\rm ath}(\bar{x},\bar{y}) = -\frac{\partial f_{\rm ath}(\bar{x},\bar{y})}{\partial \bar{y}}. \tag{74}$$

The entropy has a contribution only from the thermal part and is given by

$$S_{\rm ni} \simeq k_B\int \frac{d\mathbf{r}}{\lambda_T^3}\left(-\frac{5}{2}f_{\rm th}(x,y) + x u_{\rm th}(x,y) - y w_{\rm th}(x,y)\right). \tag{75}$$

The Hohenberg-Kohn free energy becomes

$$F_{\rm nc}([n_{\rm nc},\Delta_{\rm nc},\Delta_{\rm nc}^*],T) \simeq \int d\mathbf{r}\left(\frac{k_BT}{\lambda_T^3}\tilde{f}_{\rm th}(u_{\rm th},w_{\rm th}) + \mathcal{E}_c k_c^3 \tilde{f}_{\rm ath}(u_{\rm ath},w_{\rm ath})\right), \tag{76}$$

where the Legendre transforms are defined as [again, the minimization may be replaced by the requirements of Eq. (74)]

$$\begin{aligned}\tilde{f}_{\rm th}(u_{\rm th},w_{\rm th}) &= \max_{x,y}[f_{\rm th}(x,y) - xu_{\rm th} + yw_{\rm th}],\\ \tilde{f}_{\rm ath}(u_{\rm ath},w_{\rm ath}) &= \max_{\bar{x},\bar{y}}[f_{\rm ath}(\bar{x},\bar{y}) - \bar{x}u_{\rm ath} + \bar{y}w_{\rm ath}],\end{aligned} \tag{77}$$

and are used with the conditions

$$\begin{aligned}&\lambda_T^3 u_{\rm th} + k_c^3 u_{\rm ath} = n_{\rm nc}, \quad 2\lambda_T^3 w_{\rm th} + 2k_c^3 w_{\rm ath} = |\Delta_{\rm nc}|,\\ &k_BT\frac{\partial\tilde{f}_{\rm th}}{\partial u_{\rm th}} = \mathcal{E}_c\frac{\partial\tilde{f}_{\rm ath}}{\partial u_{\rm ath}}, \quad k_BT\frac{\partial\tilde{f}_{\rm th}}{\partial w_{\rm th}} = \mathcal{E}_c\frac{\partial\tilde{f}_{\rm ath}}{\partial w_{\rm ath}}.\end{aligned} \tag{78}$$

Further details regarding $f_{\rm th}$ and $f_{\rm ath}$ are given in the Appendix and, for $f_{\rm th}$, also in Sec. V.

As for the Φ-DFT of Sec. III, a local Thomas-Fermi approach can be applied to the condensate amplitude Φ as well, amounting to neglecting the derivative term in Eq. (57), resulting in a completely local description.

### C. Interaction effects

A local description of the interaction effects (LDA) for the present application of DFT requires knowledge of $f_{\rm int}(n,\Phi,\Phi^*,\Delta,\Delta^*,T)$—the interaction energy density for a uniform system of density $n$, condensate amplitude Φ, and anomalous density Δ, at temperature $T$. Its derivatives will determine the potentials of the reference system, which include

$$\xi_{\rm ni}(\mathbf{r}) = \xi_{\rm ext}(\mathbf{r}) + \xi_{\rm int}(\mathbf{r}) = -\frac{\partial f_{\rm int}}{\partial\Delta^*}, \tag{79}$$

in addition to Eq. (40) for the interaction contribution to the effective potential $v_{\rm ni}$ and fictitious field $\eta_{\rm ni}$.

As in Sec. III, one may use the weakness of the interactions in order to derive a simple approximation for $f_{\rm int}$ by evaluating the interaction energy to leading order in the interaction strength $g$,

$$f_{\rm int} \simeq \frac{g}{2}(|\Phi|^4 + 4|\Phi|^2\langle\hat{\phi}^\dagger\hat{\phi}\rangle + \Phi^{*2}\langle\hat{\phi}\hat{\phi}\rangle + \Phi^2\langle\hat{\phi}^\dagger\hat{\phi}^\dagger\rangle + \langle\hat{\phi}^\dagger\hat{\phi}^\dagger\hat{\phi}\hat{\phi}\rangle), \tag{80}$$

due to the mixing of creation and annihilation operators in Eq. (60), since expectation values of the type $\langle\hat{\phi}\hat{\phi}\rangle$ no longer vanish. Similarly, Wick's theorem becomes $\langle\hat{\phi}_1^\dagger\hat{\phi}_2^\dagger\hat{\phi}_3\hat{\phi}_4\rangle = \langle\hat{\phi}_1^\dagger\hat{\phi}_2^\dagger\rangle\langle\hat{\phi}_3\hat{\phi}_4\rangle + \langle\hat{\phi}_1^\dagger\hat{\phi}_4\rangle\langle\hat{\phi}_2^\dagger\hat{\phi}_3\rangle + \langle\hat{\phi}_1^\dagger\hat{\phi}_3\rangle\langle\hat{\phi}_2^\dagger\hat{\phi}_4\rangle$. Using both $n = |\Phi|^2 + \langle\hat{\phi}^\dagger\hat{\phi}\rangle$ and $\Delta = \Phi^2 + \langle\hat{\phi}\hat{\phi}\rangle$ gives

$$f_{\rm int} \simeq \frac{g}{2}(2n^2 + |\Delta|^2 - 2|\Phi|^4). \tag{81}$$

This result can be interpreted as a triple counting of the condensate term, compensated by a double subtraction—the $|\Phi|^4$ contribution appears in the direct $(\langle\hat{\psi}_1^\dagger\hat{\psi}_4\rangle\langle\hat{\psi}_2^\dagger\hat{\psi}_3\rangle)$, the exchange $(\langle\hat{\psi}_1^\dagger\hat{\psi}_3\rangle\langle\hat{\psi}_2^\dagger\hat{\psi}_4\rangle)$, and the anomalous $(\langle\hat{\psi}_1^\dagger\hat{\psi}_2^\dagger\rangle\langle\hat{\psi}_3\hat{\psi}_4\rangle)$ term but physically should be accounted for only once. Using this approximation in Eqs. (40) and (79) for the effective potentials gives

$$\begin{aligned}v_{\rm ni}(\mathbf{r}) &\simeq v_{\rm ext}(\mathbf{r}) + 2gn(\mathbf{r}),\\ \eta_{\rm ni}(\mathbf{r}) &\simeq 2g|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}),\\ \xi_{\rm ni}(\mathbf{r}) &\simeq -\frac{g}{2}\Delta(\mathbf{r}).\end{aligned} \tag{82}$$

Substitution of this approximation into Eq. (57) gives the generalized G-P equation

$$\left(-\frac{\hbar^2\nabla^2}{2m} + v_{\rm ext} - \mu + 2gn_{\rm nc} + g|\Phi(\mathbf{r})|^2\right)\Phi + g\Delta_{\rm nc}\Phi^* = 0, \tag{83}$$

which contains an extra term involving $\Delta_{\rm nc}$[cf. Eq. (52)]. These potentials are also to be used in the Bogoliubov–de Gennes equation, Eq. (61).

This approach reproduces the equations of the Hartree-Fock-Bogoliubov method, which have been systematically derived and studied for a long time [15,44–48]. In that context, the method is intended to calculate not only the thermodynamic properties of the system, but also its excitation spectrum. It has been criticized for producing a spectrum with a gap at small wavenumbers in homogeneous systems, while it is known that the correct long-wavelength result involves a gapless linear phonon spectrum [44]. A related difficulty arises at short distances, where it is seen that $\Delta(\mathbf{r}) = \lim_{\mathbf{r}'\to\mathbf{r}}\langle\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle$ depends on the large wavenumber cutoff $k_c$ (for $T = 0$ and weak interactions, one may use the limit of $f_{\rm ath}$ discussed in the Appendix to find $n_{\rm nc}/n \sim \sqrt{na_0^3}$ and $\Delta_{\rm nc}/n \sim k_c a_0$, in agreement with the literature). As $\Delta_{\rm nc}$ involves a product of operators at essentially the same point in space, such a cutoff dependence should be accepted, and indeed, the nature of the point interaction should be expected to generate a relationship between this ultraviolet divergence and long-wavelength behavior. Approximations that are designed to produce a spectrum without a gap have been studied [46,47], and more recently, a pseudopotential that allows for a rigorous treatment overcoming these difficulties (at least at zero temperature) has been suggested [50].

In the context of DFT, it may be argued that the spectrum is irrelevant as it represents a property of the reference system, which need not be shared with the interacting system. Thus, in principle, it may be claimed that A-DFT is rigorously exact, despite the presence of the gap. However, it is clear that the spectrum affects the thermodynamic properties, and that, if the reference system has properties that differ significantly from those of the interacting system, it will be difficult to find workable approximations for $F_{\rm int}$. Thus, it may be desirable to adopt the advanced pseudopotential approach for DFT [50]. This would require using a reference system with nonlocal effective potentials [i.e., introducing terms of the form $\xi(\mathbf{r},\mathbf{r}')\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')$ and $\upsilon(\mathbf{r},\mathbf{r}')\psi^\dagger(\mathbf{r})\psi(\mathbf{r}')$ into the Hamiltonian] with $\xi_{\rm ext} = \upsilon_{\rm ext} = 0$ but $\xi_{\rm ni},\upsilon_{\rm ni} \neq 0$ in close analogy with the foregoing derivation, and is beyond the scope of this paper.

## V. THE UNIFORM-SYSTEM WEAK-INTERACTIONS LIMIT

Having introduced both Φ-DFT and A-DFT, a discussion of applications is in order. Essentially all applications are beyond the scope of this paper, but one exercise which is particularly revealing will be presented here: the weak-interactions limit of homogeneous systems. Strictly speaking, this is not an application of DFT, and should be viewed as an application in thermodynamic perturbation theory. It will have relevance to the LDA, which (as noted before) relies on knowledge of the properties of uniform systems.

The Thomas-Fermi approach is accurate (not an approximation) for homogeneous systems. Hence, the results of the Thomas-Fermi sections, Secs. III B 1 and IV B 1, are directly applicable. Similarly, the lowest-order linear term in the interaction strength $g$ has been given previously for both Φ-DFT and A-DFT. The discussion here pertains to a finite temperature not too near either the BEC transition or $T = 0$, and, thus, the interactions are treated as perturbing a noninteracting Bose-Einstein-condensed system.

### A. Two-fluid method

Applying the Φ-DFT of Sec. III to a uniform system, one drops the gradient terms in the G-P equation (52) and solves it in conjunction with Eq. (46) in the $g \to 0$ limit. The external potential is set to 0, and the $x \to 0$ limit of the thermodynamic function $f$ defined in Eq. (45) is pertinent (cf. Fig. 2),

$$f(x) = -\zeta(5/2) + \zeta(3/2)x - \frac{4\sqrt{\pi}}{3}x^{3/2} + O(x^{5/2}), \tag{84}$$

giving

$$u = f'(x) = \zeta(3/2) - 2\sqrt{\pi}x^{1/2} + O(x^{3/2}), \tag{85}$$

where $x = (2gn - \mu)/k_BT$ from Eq. (51) and $u = \lambda_T^3 n_{\rm th}$. This relation between the effective potential and the density may be inverted as

$$x = \frac{\delta u^2}{4\pi} + O(\delta u^4), \tag{86}$$

where the notation $\delta u = \zeta(3/2) - u$ has been used and the Legendre transformed Helmholtz free energy is, in dimensionless form

$$\tilde{f}(u) = -\zeta(5/2) + \frac{\delta u^3}{12\pi} + O(\delta u^5). \tag{87}$$

Thus, the Hohenberg-Kohn free energy per unit volume of the uniform system, including the interaction terms to leading order in $g$ from Eq. (49), is

$$\frac{F_{\rm HK}([n,\Phi,\Phi^*],T)}{V} \simeq \frac{k_BT}{\lambda_T^3}\tilde{f}(\lambda_T^3(n - \Phi^*\Phi)) + \frac{g}{2}[2n^2 - (\Phi^*\Phi)^2]. \tag{88}$$

Although it is straightforward to apply the self-consistent Kohn-Sham equations to this system, [which, here, amounts to using, e.g., Eq. (85)] a more physically transparent discussion will result from following a minimum-energy path closer in spirit to the Hohenberg-Kohn approach. Thus, the physical requirement that the external auxiliary field vanish, $\eta_{\rm ext} = \partial F_{\rm HK}/\partial\Phi^* = 0$, will be imposed by minimizing the free energy of Eq. (88) with respect to $\Phi^*$ at a given overall density $n$. From Eq. (87), this amounts to minimization of

$$\frac{\delta u^3}{6\pi} - \frac{g}{k_BT\lambda_T^3}\left[\lambda_T^3 n - \zeta(3/2) + \delta u\right]^2, \tag{89}$$

with respect to $\delta u = \lambda_T^3(|\Phi|^2 - n) + \zeta(3/2)$, with $\delta u \geqslant 0$, but small. At $g = 0$, one finds $\delta u = 0$ or $|\Phi_0|^2 = n - \zeta(3/2)\lambda_T^{-3}$, whereas, for small $g$, one finds $\delta u \simeq 2\sqrt{\frac{\pi g}{k_BT}|\Phi_0|^2}$. This gives

$$|\Phi|^2 \simeq |\Phi_0|^2 + 2\lambda_T^{-3}\sqrt{\frac{\pi g}{k_BT}|\Phi_0|^2}, \tag{90}$$

a result whose accuracy should be questioned, as discussed later. Note that the particularly soft $\delta u^3$ behavior of $\tilde{f}(u)$, corresponding to the nonanalytic cusp in $f(x)$ at $x = 0$, has resulted in a sensitivity to interactions, which is displayed by the sharp $\sqrt{g}$ dependence of the condensate amplitude (in other words, the position of a shallow minimum is easily changed by a perturbation that is sloped in that region). It is straightforward but not particularly illuminating to obtain additional thermodynamic results at this level of approximation (e.g., to find the relationship between the chemical potential $\mu$ and the overall density $n$).

### B. Bogoliubov method

Application of the A-DFT of Sec. IV to the present problem requires expanding the thermodynamic functions defined in Eq. (70) at small values of their arguments [see the Appendix, Eqs. (A4) and (A5)],

$$f_{\rm th}(x,y) = -\zeta(5/2) + \zeta(3/2)x - \frac{2\sqrt{\pi}}{3}[(x+2y)^{3/2} + (x-2y)^{3/2}] + O(x^2), \tag{91}$$

where the requirement $0 \leqslant y \leqslant x/2$ is used to drop $O(y^2)$ contributions. A comparison with Eq. (84) already is interesting at this stage: Clearly, setting the anomalous potential to zero, $y = 0$, reproduces the Φ-DFT result, but taking the Bogoliubov spectrum with a vanishing gap corresponds here to setting $y = x/2$ and results in an extra factor of $\sqrt{2}$ in the $x^{3/2}$ term. The expansion of $f_{\rm ath}$ begins with $O(x^2)$ terms, Eq. (A9), and, therefore, the athermal component does not affect the results to leading order in $g$.

The scaled density and anomalous density are

$$u_{\rm th} = \frac{\partial f_{\rm th}}{\partial x} \simeq \zeta(3/2) - \sqrt{\pi}(\sqrt{x+2y} + \sqrt{x-2y}), \tag{92}$$

and

$$w_{\rm th} = -\frac{\partial f_{\rm th}}{\partial y} \simeq 2\sqrt{\pi}(\sqrt{x+2y} - \sqrt{x-2y}), \tag{93}$$

and inverting these relationships gives

$$x \simeq \frac{1}{4\pi}\left(\delta u_{\rm th}^2 + \frac{1}{4}w_{\rm th}^2\right), \qquad y \simeq \frac{1}{8\pi}\,\delta u_{\rm th}\, w_{\rm th}, \tag{94}$$

where, again, $\delta u_{\rm th} = \zeta(3/2) - u_{\rm th}$. The result for the Hohenberg-Kohn free energy is

$$\tilde{f}_{\rm th}(u_{\rm th}, w_{\rm th}) = -\zeta(5/2) + \frac{1}{4\pi}\left(\frac{1}{3}\,\delta u_{\rm th}^3 + \frac{1}{4}w_{\rm th}^2\,\delta u_{\rm th}\right) + O\left(\delta u_{\rm th}^4\right). \tag{95}$$

The overall free energy, including the interaction terms to leading order, Eq. (81), excluding the athermal contribution, is

$$\frac{F_{\rm HK}(n,\Phi,\Phi^*,\Delta,\Delta^*,T)}{V} \simeq k_B T\lambda_T^{-3}\tilde{f}_{\rm th}\left(\lambda_T^3(n-|\Phi|^2),\lambda_T^3|\Delta-\Phi^2|\right) + \frac{g}{2}(2n^2+|\Delta|^2-2|\Phi|^4). \quad (96)$$

In the present case, both fictitious potentials $\eta$ and $\xi$ must vanish (i.e., the free energy is to be minimized with respect to both $\Phi$ and $\Delta$). In dimensionless terms, this corresponds to minimization of

$$\frac{1}{2\pi}\left(\frac{1}{3}\delta u_{\rm th}^3+\frac{1}{4}\delta u_{\rm th}\, w_{\rm th}^2\right) + \frac{g}{k_B T\lambda_T^3}\left(\left[\lambda_T^3 n-\zeta(3/2)+\delta u_{\rm th}-\frac{w_{\rm th}}{2}\right]^2 - 2\left[\lambda_T^3 n-\zeta(3/2)+\delta u_{\rm th}\right]^2\right), \quad (97)$$

with respect to both $\delta u_{\rm th}$ and $w_{\rm th}$ (in principle, an arbitrary phase factor could be associated with the $\frac{w_{\rm th}}{2}$ term, reflecting the relative phase between $\Delta_{\rm nc}$ and $\Phi^2$, but the sign used here is clearly optimal). The minimization requires

$$\delta u_{\rm th}^2+\frac{1}{4}w_{\rm th}^2 \simeq \frac{4\pi g}{k_B T\lambda_T^3}\left(\lambda_T^3 n-\zeta(3/2)+\delta u_{\rm th}+\frac{w_{\rm th}}{2}\right),$$
$$\delta u_{\rm th}\, w_{\rm th} \simeq \frac{4\pi g}{k_B T\lambda_T^3}\left(\lambda_T^3 n-\zeta(3/2)+\delta u_{\rm th}-\frac{w_{\rm th}}{2}\right). \quad (98)$$

To leading order in $g$, we may use $\delta u_{\rm th}\simeq 0$ and $w_{\rm th}\simeq 0$ in the RHS, resulting in $\delta u_{\rm th}\simeq w_{\rm th}/2\simeq\sqrt{\frac{2\pi g}{k_B T\lambda_T^3}[\lambda_T^3 n-\zeta(3/2)]}$, or

$$|\Phi|^2\simeq|\Phi_0|^2+\lambda_T^{-3}\sqrt{\frac{2\pi g}{k_B T}}|\Phi_0|^2, \quad (99)$$

together with a similar contribution to $\Delta_{\rm nc}$ (at this order, we have $x=2y$). Here, the interaction-dependent correction to the condensate fraction is a factor of $\sqrt{2}$ smaller than the result of Sec. V A, Eq. (90). This discrepancy will be discussed in Sec. V C. The present result, which includes the effects of the anomalous density through $w$, is in accordance with the literature [47] (recall that $g\simeq 4\pi\hbar^2 a_0/m$ and $\lambda_T=\sqrt{2\pi\hbar^2/mk_B T}$).

### C. Comparison of the two-fluid and Bogoliubov reference systems

It is at first surprising that the two methods being discussed lead to two different results for the leading-order correction to the condensate fraction of a uniform BEC. After all, both methods are based on a straightforward expansion in the small parameter $g$, within a thermodynamic framework, which is, in principle, exact. The only source of error can be the neglect of terms in the interaction energy $f_{\rm int}$, which are of higher order in $g$. The following paragraphs display these terms explicitly.

Clearly, the level of accuracy used in the A-DFT description can be imported into $\Phi$-DFT by choosing the appropriate form for $f_{\rm int}(n,\Phi,\Phi^*)$. In fact, it is obvious that simply dropping the anomalous term in Eq. (97), setting $w_{\rm th}=0$, reduces it to Eq. (89). However, the proper procedure is to minimize over $w_{\rm th}$, which corresponds to imposing the condition $\xi=0$ (i.e., to requiring the vanishing of the anomalous potential rather than the $w_{\rm th}$ contribution to the anomalous density). From the second line in Eq. (98), this leads (to leading order in $g$) to

$$w_{\rm th}\simeq\frac{4\pi g}{k_B T\lambda_T^3}\frac{\lambda_T^3 n-\zeta(3/2)}{\delta u_{\rm th}}. \quad (100)$$

Introducing this into Eq. (97) gives

$$\frac{1}{6\pi}\delta u_{\rm th}^3-\frac{g}{k_B T\lambda_T^3}\left(\lambda_T^3 n-\zeta(3/2)+\delta u_{\rm th}\right)^2 - 2\pi\left(\frac{g}{k_B T\lambda_T^3}\right)^2\frac{\left(\lambda_T^3 n-\zeta(3/2)\right)^2}{\delta u_{\rm th}}, \quad (101)$$

where terms up to second order in $g$ have been retained (one can check *a posteriori* that the neglected terms are indeed small). Minimization of this, to leading order, amounts to the requirement that

$$\left(\delta u_{\rm th}^2-\frac{2\pi g}{k_B T\lambda_T^3}\left[\lambda_T^3 n-\zeta(3/2)\right]\right)^2=0, \quad (102)$$

which displays how dropping terms of second order in $g$ leads to a doubling of the result for $\delta u_{\rm th}^2$. Thus, it is clarified that a weakly interacting BEC system is situated near a singular point, associated physically with a completely full thermal cloud, i.e., $u_{\rm th}=\zeta(3/2)$. At this special point, terms that are of second order in the weak interaction parameter $g$ are not relatively small, because they are divergent, with the small quantity $\delta u_{\rm th}$ appearing in the denominator.

## VI. SUMMARY AND OUTLOOK

The thermodynamic approach (summarized in Sec. II) provides a general method for generating DFTs for bosonic systems in thermal equilibrium at finite temperature, and has been used to derive the equations of $\Phi$-DFT (Sec. III) and of A-DFT (Sec. IV). The different DFTs use, as references, different types of Kohn-Sham systems, which are subject to different fictitious potentials. The reference systems have quadratic soluble Hamiltonians, and the interaction effects are to be included via an LDA. The latter must be based on knowledge of the free energy of interacting homogeneous systems, which are subject to the fictitious potentials. For $\Phi$-DFT, knowledge of the free energy of a homogeneous interacting system as a function of $\mu$, $T$, and $\eta$ is required in order to supply $f_{\rm int}(n,\Phi,\Phi^*,T)$, and, for A-DFT, a $\xi$ field must also be allowed for. This type of information is generally available only for the leading order in the interaction parameter $g$. In this limit, our results for $\Phi$-DFT generalize the two-fluid approach [41] for inhomogeneous systems, and the results for A-DFT reproduce the Hartree-Fock-Bogoliubov model. As has occurred for electronic systems, we anticipate that the necessary results beyond the leading order will be generated using quantum Monte Carlo techniques. Such techniques have been developed for Bose-Einstein-condensed systems [55], but, as the fictitious potentials $\eta$ and $\xi$ break particle-number

conservation, different variants of the techniques may need to be developed to meet this goal.

It is of interest to compare Φ-DFT and A-DFT to the attempt made in Ref. [36] to apply DFT to BEC systems, using the standard approach to DFT rather than the thermodynamic one. In this reference, only two functional variables were used—$n$ and Φ, as in Φ-DFT—but the reference or Kohn-Sham system chosen employed a Bogoliubov-type treatment, similar to that used in A-DFT. Correspondingly, the Hamiltonian of the reference system depends not only on the potentials used, but also on the (anomalous) density, which is to be calculated self-consistently. This represents a difficulty that the present thermodynamic derivation avoids.

In comparing the two DFT methods, it was found that, in the limit of homogeneous weakly interacting systems at finite temperatures, Φ-DFT (or the two-fluid method) does not correctly reproduce the leading-order correction to the condensate density, and that this flaw can be corrected by including higher-order terms in $f_{\rm int}$. This is due to the extreme sensitivity of the corresponding energy-minimization problem: (a) Terms of order $g$ in the energy cause a shift in the minimizing value of Φ, which is of order $\sqrt{g}$, and (b) the second-order term in $f_{\rm int}$ is divergent, having an $O(\sqrt{g})$ denominator, thus, contributing to $O(g^{3/2})$ in the energy and to a significant change in the $O(\sqrt{g})$ correction to Φ. The higher-order terms in $f_{\rm int}$ for Φ-DFT were, in this case, obtained from a first-order A-DFT calculation, which amounts to reexpressing the Hartree-Fock-Bogoliubov model as a minimization problem (Sec. V).

The comparison just mentioned demonstrates the advantages of A-DFT—it uses a reference system that is much closer in its behavior to the fully interacting system, and, therefore, the approximation introduced is much less significant. It is reasonable to expect that this advantage will be significant for inhomogeneous systems as well. Thus, obtaining the requisite data for homogeneous interacting systems as a function of both $\eta$ and $\xi$ is called for. As an interim step, applications of Φ-DFT, for which strong-interaction corrections to $f_{\rm int}$ could more easily be acquired, should also be considered.

## ACKNOWLEDGMENTS

The authors wish to thank Y. Avishai for the role he played in initial stages of this project. This work was supported, in part, by grants from the U.S.-Israel Binational Science Foundation (Grant No. 2006212), the Israel Science Foundation (Grant No. 29/07), and the James Franck German-Israel Binational Program.

## APPENDIX: INTEGRALS FOR THE THOMAS-FERMI APPROXIMATION OF A-DFT

In Sec. IV, Eq. (70), integrals corresponding to the thermodynamic functions $f_{\rm th}$ and $f_{\rm ath}$ were introduced, and in Sec. V, the need to evaluate these integrals in the limit corresponding to weak interactions arose. The details of the evaluations are presented here.

For the thermal contribution, integration of Eq. (71) by parts gives

$$f_{\rm th}(x,y)=\frac{-8}{3\sqrt{\pi}}\int_0^\infty \frac{\sqrt{(q^2+x)^2-4y^2}}{\exp\left(\sqrt{(q^2+x)^2-4y^2}\right)-1} \times \frac{q^4(q^2+x)\,dq}{(q^2+x)^2-4y^2}. \tag{A1}$$

The second factor is separated as

$$\frac{q^4(q^2+x)}{(q^2+x)^2-4y^2}=q^2-x+\frac{1}{2}\left(\frac{(x-2y)^2}{q^2+x-2y}+\frac{(x+2y)^2}{q^2+x+2y}\right), \tag{A2}$$

where the term $q^2-x$ diverges with $q$, and the remaining terms converge rapidly. This may be used to write $f_{\rm th}=I_1+I_2$, with the integrals $I_1$ and $I_2$ involving the divergent and convergent terms, respectively.

At small $x$ and $y$, the square-root term can be expanded as

$$\sqrt{(q^2+x)^2-4y^2}=q^2+x+O(x^2), \tag{A3}$$

where, as before, terms of order $y^2$ are included in $O(x^2)$ because of the limitation $x\geqslant 2y\geqslant 0$. One finds

$$I_1=\frac{-8}{3\sqrt{\pi}}\int_0^\infty \frac{q^2+x}{\exp(q^2+x)-1}(q^2-x)\,dq+O(x^2) =-\zeta(5/2)+\zeta(3/2)x+O(x^2) \tag{A4}$$

(note cancellation of terms at order $x^{3/2}$) and

$$I_2=\frac{-4}{3\sqrt{\pi}}\int_0^\infty\left(\frac{(x-2y)^2}{q^2+x-2y}+\frac{(x+2y)^2}{q^2+x+2y}\right)dq+O(x^2) =\frac{-2\sqrt{\pi}}{3}[(x-2y)^{3/2}+(x+2y)^{3/2}]+O(x^2), \tag{A5}$$

where, in the last equation, $(q^2+x)/(e^{q^2+x}-1)$ was approximated by unity because the remaining factors are already of relatively high order in $x$ and are small when $q^2\gg x$. These results are used in Sec. V, Eq. (91).

For the athermal contribution, one may rewrite Eq. (72) as

$$f_{\rm ath}(\bar{x},\bar{y})=-\frac{4}{\sqrt{\pi}}\bar{y}^2+\frac{2}{\sqrt{\pi}}\int_0^1[(\sqrt{(q^2+\bar{x})^2-4\bar{y}^2}-q^2-\bar{x}) \times q^2+2\bar{y}^2]\,dq, \tag{A6}$$

where the integral can be continued to infinity without divergence, as can be seen by expanding the square root as

$$\sqrt{(q^2+\bar{x})^2-4\bar{y}^2}=q^2+\bar{x}-\frac{2\bar{y}^2}{q^2}+O(\bar{x}^3). \tag{A7}$$

Rescaling $q$ by $\sqrt{\bar{x}}$, and defining

$$h(\alpha)=\int_0^\infty\left[(\sqrt{(q^2+1)^2-\alpha}-q^2-1)q^2+\frac{\alpha}{2}\right]dq, \tag{A8}$$

where $\alpha=4\bar{y}^2/\bar{x}^2$ is a variable in the range $0\leqslant\alpha\leqslant 1$, gives

$$f_{\rm ath}(\bar{x},\bar{y})=-\frac{4}{\sqrt{\pi}}\bar{y}^2+\frac{2\bar{x}^{5/2}}{\sqrt{\pi}}h(\alpha)+O(\bar{x}^3). \tag{A9}$$

The integral $h(\alpha)$ vanishes at $\alpha = 0$ and increases with $\alpha$ to a value of $8\sqrt{2}/15$ at $\alpha = 1$. This value may be derived as

$$\int_0^\infty \left[(\sqrt{q^4+2q^2}-q^2-1)q^2+\frac{1}{2}\right] dq = \lim_{Q\to\infty} -\frac{Q^5}{5}-\frac{Q^3}{3}+\frac{Q}{2}+\int_2^{Q^2+2}\sqrt{u}(u-2)\frac{du}{2}, \tag{A10}$$

where $u = q^2 + 2$, and the result is obtained from the lower limit of the last integral. The derivative of $h$ is given by

$$h'(\alpha) = \frac{1}{2}\int_0^\infty \left(1-\frac{q^2}{\sqrt{(q^2+1)^2-\alpha}}\right) dq, \tag{A11}$$

and decreases from $h'(0) = \pi/4$ to $h'(1) = 1/\sqrt{2}$. As these values are within 10% of each other, a plot of $h$ is very nearly a straight line and is not included. It is easily seen that $h'(\alpha) = \pi/4 - (\pi/64)\alpha + O(\alpha^2)$ for small $\alpha$, whereas, $h'(\alpha) = 1/\sqrt{2} - (1/16\sqrt{2})(1-\alpha)\ln(1-\alpha) + O(1-\alpha)$ near $\alpha = 1$, where the logarithm arises from the $1/q$ behavior of the integrand for $(1-\alpha) \ll q^2 \ll 1$. This motivates the approximation,

$$h(\alpha) \simeq c_1\alpha + c_2\alpha^2 + c_3\alpha^3 + c_4\alpha^4 + \check{c}(1-\alpha)^2\ln(1-\alpha), \tag{A12}$$

where the coefficients $c_1 = \frac{1}{4}\pi + \frac{1}{64}\sqrt{2} \simeq 0.80750$, $c_2 = -\frac{1}{128}(\pi + 3\sqrt{2}) \simeq -5.7689 \times 10^{-2}$, $c_3 = \frac{49}{30}\sqrt{2} - \frac{47}{64}\pi \simeq 2.775 \times 10^{-3}$, $c_4 = (\frac{1}{2} - \frac{1}{128})\pi - (\frac{11}{10} - \frac{1}{128})\sqrt{2} \simeq 1.6663 \times 10^{-3}$, and $\check{c} = \frac{1}{64}\sqrt{2} \simeq 2.2097 \times 10^{-2}$ are chosen so as to reproduce the calculated properties. Numerical integration of Eq. (A8) (evaluation of the integrand at large $q$ requires some care) shows that the maximum error in this approximation is less than $5 \times 10^{-5}$. As the cutoff scale is large, $\bar{x}$ and $\bar{y}$ typically are small, and such attention to the small-$\bar{x}$-and-$\bar{y}$ limit is appropriate.


[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell , Science **269**, 198 (1995).
[2] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).
[3] K. B. Davis, M.-O. Mewes, M. A. Joffe, M. R. Andrews, and W. Ketterle, Phys. Rev. Lett. **74**, 5202 (1995); K. B. Davis, M.-O. Mewes, M. R Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *ibid.* **75**, 3969 (1995).
[4] S. Inouye *et al.*, Nature (London) **392**, 151 (1998).
[5] S. L. Cornish, N. R. Claussen, J. L. Roberts, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. **85**, 1795 (2000); J. L. Roberts, N. R. Claussen, S. L. Cornish, E. A. Donley, E. A. Cornell, and C. E. Wieman, *ibid.* **86**, 4211 (2001); E. A. Donley, N. R. Claussen, S. L. Cornish, J. L. Roberts, E. A. Cornell, and C. E. Wieman, Nature (London) **412**, 295 (2001).
[6] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. **92**, 040403 (2004).
[7] L. Deng *et al.*, Nature (London) **398**, 218 (1999).
[8] M. Trippenbach, K. Góral, K. Rzazewski, B. Malomed and Y. B. Band, J. Phys. B **33**, 4017 (2000).
[9] Y. B. Band, J. P. Burke, Jr., A. Simoni, and P. S. Julienne, Phys. Rev. A **64**, 023607 (2001).
[10] A. P. Albus, F. Illuminati, and M. Wilkens, Phys. Rev. A **67**, 063606 (2003).
[11] G. Modugno, G. Ferrari, G. Roati, R. J. Brecha, A. Simoni, and M. Inguscio, Science **294**, 1320 (2001); G. Modugno, G. Roati, F. Riboli, F. Ferlaino, R. J. Brecha, and M. Inguscio, *ibid.* **297**, 2240 (2002).
[12] H. Hu and X.-J. Liu, Phys. Rev. A **68**, 023608 (2003).
[13] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[14] For alkali atoms, the intermolecular potential scales asymptotically as $V(r) = -C_6/r^6$, and the range of the interaction $r_0$ can be taken as the van der Waals length $r_0 = (mC_6/\hbar^2)^{1/4}$. The condition then reads $n^{-1/3} \gg r_0$.
[15] F. Dalfovo *et al.*, Rev. Mod. Phys. **71**, 463 (1999).
[16] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999).
[17] N. Argaman and G. Makov, Am. J. Phys. **68**, 69 (2000).
[18] K. Capelle, Braz. J. Phys. **36**, 1318 (2006).
[19] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[20] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[21] N. D. Mermin, Phys. Rev. **137**, A1441 (1965).
[22] L. J. Bartolotti, Phys. Rev. A **26**, 2243 (1982); E. K. U. Gross and R. M. Dreizler, in *Density Functional Methods in Physics*, edited by R. M. Dreizler and J. Providencia (Plenum, New York, 1985).
[23] E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).
[24] G. Vignale and W. Kohn, Phys. Rev. Lett. **77**, 2037 (1996).
[25] L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. **60**, 2430 (1988).
[26] C. Speicher, R. M. Dreizler, and E. Engel, Ann. Phys. (San Diego) **213**, 312 (1992).
[27] J. S. Rowlinson and F. L. Swinton, *Liquids and Liquid Mixtures*, 3rd ed. (Butterworth Scientific, London, 1982); H. T. Davis, *Statistical Mechanics of Phases, Interfaces, and Thin Films*, (VCH, New York, 1996).
[28] K. Capelle and L. N. Oliveira, Phys. Rev. B **61**, 15228 (2000); Europhys. Lett. **49**, 376 (2000).
[29] P. C. Hohenberg and P. C. Martin, Ann. Phys. (NY) **34**, 291 (1965).
[30] J. Dupont-Roc, M. Himbert, N. Pavloff, and J. Treiner, J. Low Temp. Phys. **81**, 31 (1990).
[31] N. Argaman and G. Makov, Phys. Rev. B **66**, 052413 (2002).
[32] E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).
[33] O. Gunnarsson and B. I. Lundqvist, Phys. Rev. B **13**, 4274 (1976); see also A. Görling, Phys. Rev. Lett. **85**, 4229 (2000).
[34] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).
[35] G. D. Mahan, Comments Condens. Matter Phys. **16**, 333 (1994).
[36] A. Griffin, Can. J. Phys. **73**, 755 (1995).

[37] G. S. Nunes, J. Phys. B **32**, 4293 (1999).
[38] For an example, see A. Banerjee and M. P. Singh, Phys. Rev. A **73**, 033607 (2006).
[39] Y. E. Kim and A. L. Zubarev, Phys. Rev. A **67**, 015602 (2003).
[40] J. Brand, J. Phys. B **37**, S287 (2004).
[41] A. Minguzzi, S. Conti, and M. P. Tosi, J. Phys. Condens. Matter **9**, L33 (1997).
[42] M. Zawada *et al.*, J. Phys. B **41**, 241001 (2008).
[43] D. A. W. Hutchinson, E. Zaremba, and A. Griffin, Phys. Rev. Lett. **78**, 1842 (1997). The equation for the condensate here is the same as that in Ref. [41], but the treatment of the thermal cloud is more advanced.
[44] See, e.g., A. Griffin, Phys. Rev. B **53**, 9341 (1996).
[45] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957); T. D. Lee, K. Huang, and C. N. Yang, *ibid.* **106**, 1135 (1957).
[46] S. T. Beliaev, Sov. Phys. JETP **7**, 289 (1958).
[47] V. N. Popov, *Functional Integrals in Quantum Field Theory and Statistical Physics* (Reidel, Dordrecht, 1983).
[48] J.–P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Boston, 1985).
[49] J. Harris, Phys. Rev. A **29**, 1648 (1984).
[50] M. Olshanii and L. Pricoupenko, Phys. Rev. Lett. **88**, 010402 (2001).
[51] See, e.g., note 13 in Ref. [31].
[52] N. N. Bogoliubov, J. Phys. (USSR) **11**, 23 (1947). See also Ref. [48].
[53] A. L. Fetter, Ann. Phys. (NY) **70**, 67 (1972); *Theory of a Dilute Low Temperature Bose Condensate*, in Proceedings of the International School of Physics (Enrico Fermi) Course Cxl: Varenna on Lake Como Villa Monastero, Italy, 1998 (IOS, Amsterdam, 1998); e-print arXiv:cond-mat/9811366v1.
[54] For every solution $(u_j, v_j)$ with positive energy $\mathcal{E}_j$, Eq. (61) possesses a solution $(v_j^*, u_j^*)$ with negative energy $-\mathcal{E}_j$, as discussed in Ref. [53]. These solutions, when added to the expression for the field operator, Eq. (60), reproduce terms arising from positive energies.
[55] See, e.g., W. Krauth, Phys. Rev. Lett. **77**, 3695 (1996).